The American Ceramic Society

2nd Global Forum on Advanced Materials and Technologies for Sustainable Development (GFMA-2)

and

4th International Conference on Innovations in Biomaterials, Biomanufacturing, and Biotechnologies (Bio-4)

ABSTRACT BOOK

July 21–26, 2019
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Introduction

This volume contains abstracts for over 450 presentations during the 2nd Global Forum on Advanced Materials and Technologies for Sustainable Development (GFMAT-2) and the 4th International Conference on Innovations in Biomaterials, Biomanufacturing, and Biotechnologies (Bio-4) in Toronto, ON, Canada. The abstracts are reproduced as submitted by authors, a format that provides for longer, more detailed descriptions of papers. The American Ceramic Society accepts no responsibility for the content or quality of the abstract content. Abstracts are arranged by day, then by symposium and session title. An Author Index appears at the back of this book. The Meeting Guide contains locations of sessions with times, titles and authors of papers, but not presentation abstracts.

How to Use the Abstract Book

Refer to the Table of Contents to determine page numbers on which specific session abstracts begin. At the beginning of each session are headings that list session title, location and session chair. Starting times for presentations and paper numbers precede each paper title. The Author Index lists each author and the page number on which their abstract can be found.

GFMAT-2 abstracts: pages 9 - 81
Bio-4 abstracts: pages 81 - 107

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Monday, July 22, 2019

Plenary Session

Room: Salon A/B

Session Chairs: Tatsuki Ohji, National Institute of Advanced Industrial Science and Technology (AIST); Roger Narayan, NC State University

8:30 AM

(PLEN-001-2019) Optimizing Bioactive Scaffolds: Cellular Response to Calcium Phosphate Composition and Architecture

S. M. Best*[1]

1. University of Cambridge, Department of Materials Science, United Kingdom

There have been a number of examples of successful translation of bioceramics research into clinical products over the past 40 years. In the field of orthopaedic surgery, the development of calcium phosphates has shown particular potential, due to their similarity with the chemical composition of bone mineral. Hydroxyapatite ($Ca_{10}(PO_4)_6(OH)_2$) has been of particular interest due to the ability to control composition by making chemical substitutions in the crystal lattice, which encourage bone repair. It is understood that even small changes in elemental- and phase "impurity" content can influence the biological response to the implant. Going forward, the field of tissue engineering (in bone grafting, for example) relies on the supply of high quality three dimensional scaffolds and their architecture contributes significantly to performance, This presentation will review historic and recent developments to understand the control of physical and chemical characteristics of bioactive ceramics for optimised biological response.

9:10 AM

(PLEN-002-2019) Fourth Industrial Revolution and Its Impact on Sustainable Societal Development

M. Singh*[1]

1. World Academy of Ceramics, Italy

The dawn of the fourth industrial revolution has ushered in a new era in the development of advanced materials, cutting edge technologies, and innovative products, which are affecting our lives in many ways. While the discovery of new materials has been known to culminate in major turning points in human history, these developments have also started a new era in manufacturing and production leading to different industrial revolutions during the last century. The transformative impact and functional manifestation of new materials have been demonstrated in every historical era by their integration into new products and systems. The rapidly increasing global population and higher demand of products is leading to a dramatic increase in the consumption of resources and rate of pollution creating the risk of irreversible changes in the ecosystem. The fourth industrial revolution builds and extends the impact of digitization in new and unanticipated ways leading to more efficient production and resource utilization. It is crucial for global development and economic competitiveness providing innovative sustainable development solutions to address future societal needs. This presentation will cover wide ranging resource sustainability topics and identify key challenges and opportunities for various technologies including AI, machine learning, and big data in sustainable development.

10:10 AM

(PLEN-003-2019) Biofunctionalization: A New Direction for Bioceramics Research

X. Zhang*[1]

1. Sichuan University, National Engineering Research Center for Biomaterials, China

With the progress in modern medicine, repair and replacement of tissue or organ has entered a new stage – to regenerate a living tissue or organ. Conventional wisdom believes that traditional bioceramics cannot meet this requirement, and only active biological substances can induce tissue regeneration. However, we found and demonstrated in the 1990s that bioceramics could induce the regeneration or formation of damaged/injured bone tissue by optimizing their design without the addition of living cells or growth factors. Based on this research, an osteoinductive bioceramics has been developed and has been successfully used in approximately 300,000 clinical cases. Further studies have shown that a nano CaP bioceramics can selectively regulate apoptosis or proliferation of cells. When the bone tumor or melanoma cells were co-cultured with normal cells, such as osteoblasts and fibroblasts, in the medium with nano bioceramics, we found that the apoptosis of tumor cells but the proliferation of the normal cells. The findings suggest that bioceramics may have the potential to treat diseases such as tumors and osteoporosis. Animal and clinical trials have been conducted and are showing good results. The report shows advances in the biofunctionalization of bioceramics, which may provide a revolutionary approach to regenerate tissue or organ by inanimate biomaterials.

10:50 AM

(PLEN-004-2019) From Volta to Solar Impulse: A battery journey

C. Delmas*[1]

1. Université Bordeaux, ICMCB-CNRS, France

From 30 years, the development of lithium-ion batteries has considerably changed your life. The gain in specific energy has allowed the development of mobile devices which are now used by billions of people. Today, the new goals concern the development of Electrical Vehicle and the storage of renewable energy. This requires very high energy batteries, 10^4 to 10^5 larger than the smartphone ones. The battery life time, the material availability and the price are now the main parameters which need to be considered. For mobile applications lithium-ion batteries seem to remain the best ones, while for stationary applications Na-ion batteries are very promising thanks the Na availability and its low the price. In this challenge the materials of tomorrow for the electrodes and the electrolyte have to be discovered and optimized. This presentation will give a general overview of the basics problems which have to be solved with a special focus on layered materials which seems now the most promising ones. Even if the batteries concern electrochemistry, the materials problems have to be considered from solid state chemistry. Now electrochemistry is a new tool for the solid state chemist. Several examples will be presented from this viewpoint.

11:30 AM

(PLEN-005-2019) Porous Calcium Polyphosphates: Biodegradable Bone Substitutes and Beyond

R. Pilliar*[1]

1. University of Toronto, Faculty of Dentistry, Canada

Porous biodegradable calcium polyphosphate (CPP) implants are being studied for use in repair of skeletal defects due to disease, trauma or congenital abnormalities. CPP degrades *in vivo* releasing Ca^{2+} and PO_4^{3-} ions that, if released at an appropriate rate, can serve as bone defect substitutes either in particulate or porous bulk form. Porous bulk substitutes can be custom-made to desired form using a novel additive manufacture + post-AM annealing treatment to allow fabrication of precisely-formed implants for press-fitting into defect sites where they become fixed through bone ingrowth with gradual resorption of CPP resulting, in time, in defect repair through new bone *regeneration*. For repair of synovial joints involving degraded articular cartilage and subchondral bone, novel biphasic implants are made with articular cartilage, formed *in vitro* by cell culture methods, attached to porous CPP substrates. The biphasic implants can be fitted into defect sites and in time will result in repair as a result of new tissue (cartilage and bone) *regeneration*. This approach can be extended to whole joint *regeneration* of certain joints thereby potentially offering an alternative to current practice of joint replacement using metal, ceramic, polymer implant components. The novel biphasic CPP-cartilage implants offer the possibility of *regeneration* rather than *replacement* of degraded tissues.

G1: Powder Processing Innovation and Technologies for Advanced Materials and Sustainable Development

Novel Shaping, Forming, and Sintering Technology, including Additive Manufacturing

Room: Trinity II

Session Chairs: Makio Naito, JWRI, Osaka University; Jingxian Zhang, Shanghai Institute of Ceramics, Chinese Academy of Sciences

1:20 PM

(GFMAT-001-2019) Process technology and applications of Basalt fiber reinforced SiOC Composites as UD-profiles (Invited)

R. Gadow*[1]; P. Weichand[1]

1. Institute for Manufacturing Technologies of Ceramic Components and Composites, University of Stuttgart, Germany

Promising lightweight composite materials, bridging the gap between PMC and CMC, are manufactured as polymer derived ceramics by the use of polysiloxanes and basalt fibers. Such competitive free formable Hybrid Composites are capable for lightweight applications in a temperature range between 300 and 850 °C and short time exposure up to over 1000 °C, even in oxidative atmosphere. The special densification effect in conical extrusion nozzles under sumultaneous curing and heating of pulltruded profiles leads to dense composite structures with high fiber volume content. The pultruded products feature high strength and toughness at high production rates and reasonable cost. Sub micron fine filler powders have been introduced to further reduce the shrinkage of the matrix as well as subsequent re- impregnation by low vicosity resins. These attributes enable the Hybrid Composite as ideal material for fire retardant applications in automotive and public transportation, as well as in fire protection systems in electrical and civil engineering applications. Moreover, the Hybrid Composite show excellent tribological properties. An adjustable value of hardness and coefficient of friction open up a wide variety of friction applications. A detailed view on the manufacturing processes and (raw-) material characterization will be given and already proven industrial applications are introduced.

1:50 PM

(GFMAT-002-2019) Effect of multifunctional acrylate structure on in-situ solidification behavior of non-aqueous Si_3N_4 slurries induced by Michael additive reaction

M. Iijima*[1]; K. Hasegawa[1]; J. Tatami[1]

1. Yokohama National University, Graduate School of Environment and Information Sciences, Japan

In-situ solidification technique of dense non-aqueous slurries stabilized by a complex of polyethyleneimine and oleic acid (PEI-OA) through adding small amount of multifunctional acrylates is one of the promising routes to shape complex-structured ceramics. Although this system is known to have inter-particle cross-linking reaction by gentle heat-induced Michael additive reaction between multifunctional acrylates and amine segments of PEI-OA fixed on the surface of fine particles, the detailed effects of processing parameters on in-situ solidification behavior is still not well understood. Herein, we systematically report the effect of multifunctional acrylate structure on in-situ solidification behavior of PEI-OA stabilized slurries using Si_3N_4/α-terpineol slurry as a model system. Poly(ethylene glycol) dimethacrylates with different molecular weights (Mw 250, 575, 750), tetramethylol methane tetraacrylate, and dipentaerythritol hexaacrylate were selected as multifunctional acrylates having 2, 4, and 6 numbers of acryloyl groups, respectively. By monitoring the changes of storage modulus of 37 vol% Si_3N_4/α-terpineol slurries treated with different acrylates by dynamic viscoelasticity test, acrylates having longer and/or higher number of acryloyl groups found to effectively solidify the slurry.

2:10 PM

(GFMAT-003-2019) Chemical Solidification of Silica Powder Surface-activated by Mechanochemical Treatment

M. Fuji[1]; R. Nojiri*[1]; H. Razavi Khosroshahi[1]

1. Nagoya Institute of Technology, Japan

Emission of green house gases such as carbon dioxide has become a serious environmental issue in recent decades. Fabrication of ceramic materials, which usually requires a firing process at high temperatures, generates a huge amount of green house gases. To develop an eco-friendly process for ceramics manufacturing, elimination of firing process from ceramics production is necessary. In our research group, we propose a solution for this problem via a chemical solidification of inorganic powder using mechanochemical surface activation. In this method, a solid with mechanical properties comparable to sintered ceramics from inorganic powders is obtained at room temperature. Ceramics produced through this method are called "Non-firing ceramics". Non-firing process will be able to fabricate new conceptual composite and hybrid materials, because the process takes place at room temperature. In this presentation, I will introduce you to fabricate functional ceramics ceramics through the non-firing process.

2:30 PM

(GFMAT-004-2019) Enhancing toughness and strength of SiC ceramics with reduced graphene oxide by HP sintering

Y. Huang*[1]

1. Shanghai Institute of Ceramics, Chinese Academy of Sciences, China

In this paper, the silicon carbide-reduced graphene oxide (SiC/rGO) composites with different content of rGO are investigated. The hot pressing (HP) at 2100ºC for 60min under a uniaxial pressure of 40MPa resulted in a near fully-dense SiC/rGO composite. In addition, the influence of graphene reinforcement on the sintering process, microstructure, and mechanical properties (fracture toughness, bending strength, and Vickers hardness) of SiC/rGO composites is discussed. The fracture toughness of SiC/rGO composites ($7.9 MPam^{1/2}$) was strongly enhanced by incorporating rGO into the SiC matrix, which was 97% higher than the solid-state sintering SiC ceramics (SSiC) by HP. Meanwhile, the bending strength of the composites reached 625MPa, which was 17.3% higher than the reference materials (SSiC). The microstructure of the composites revealed that SiC grains were isolated by rGO platelets, which lead to the toughening of the composite through rGO pull out/debonding and crack bridging mechanisms.

Particle and Powder Design and Synthesis

Room: Trinity II

Session Chairs: Jian Luo, University of California, San Diego; Toshihiro Ishikawa, Tokyo University of Science, Yamaguchi (Sanyo-Onoda City University)

3:20 PM

(GFMAT-005-2019) Novel electrical disintegration for selective dismantling of spent products (Invited)

C. Tokoro*[1]

1. Waseda University, Japan

For sustainable usage of resources by reuse and recycling, selective dismantling technologies for spent products have been desired. The electrical disintegration is known as a grinding method to preferentially destroy different phase boundary with different conductivity and has been used to promote the liberation of ores and wastes in mineral processing and recycling. In this study, I introduce a novel electrical disintegration method which improves selectivity of disassembly by controlling electrode position, voltage and current. By this method, selective separation between thin materials became possible. For example, by disposing the electrical pulse electrodes on the positive electrode material taken out from the spent lithium ion battery and by irradiating the electric pulse once, separation between the aluminum foil and the positive electrode material particles was achieved. Besides, for the remaining cell sheets from the spent polycrystalline silicon photovoltaic module after peeled off the glass panel, selective separation of Cu/Ag wire with silicon particles from the resin layer was obtained by disposing the electrodes on the wire. This separation was achieved by selective thin wire explosion of Cu/Ag wire and peeling of silicon particles by shock wave generated by pulse arc discharge.

3:50 PM

(GFMAT-006-2019) Thermal Stability and Property of Osmium Boride Based Ceramic Compounds Synthesized by Mechanochemical Processing (Invited)

H. Lin*[1]

1. Guangdong University of Technology, School of Electromechanical Engineering, China

Transition metal borides (TMBs), like OsB_2, have been attracted great attentions due to its ultra-high bulk modulus, high stiffness, and high wear resistance. Thus, these types of TMBs have drawn great scientific interests in material community due to their potential for wide machining industry applications. It has been recognized that the preparation of high purity and homogeneous OsB_2 powders was not a trivial task via conventional processing routes. The mechanochemical synthesis approach has been studied as an alternative processing method for manufacturing compounds that are difficult or impossible to obtain by conventional techniques at room temperature. The paper will report the evolution of phase and morphology of OsB_2 powders as a function of Os/B ratio, ball size arrangements, and milling time during the high energy mechanical milling process. In addition, an engineering approach was also employed to improve the thermal stability of the ReB_2 type hexagonal OsB_2 by forming $Os_{1-x}M_xB_2$ solid solution via the addition of Re and W element. The effects of Re and W addition on the OsB_2 structure, thermal stability, and mechanical property as a function of milling time will be presented and discussed, separately. Results obtained from this research might provide engineering design and processing guidelines for the search of novel ReB_2 type hexagonal borides.

4:20 PM

(GFMAT-007-2019) Application of the eccentric stirring milling on the efficient glass recovery from photovoltaic panel

M. Nishi*[1]; Y. Tsunazawa[1]; S. Kato[3]; M. Harita[2]; S. Owada[1]; C. Tokoro[1]

1. Waseda University, Japan
2. Harita Metal Co., Ltd., Japan
3. The Glass Recycling Committee of Japan, Japan

Photovoltaic (PV) panels are widely used in the world, and the consumption of PV panels has been exponentially increasing. However, the recycling system of PV panels has not been established. For the growing amount of wasted PV panels in the near future, it is strongly required to develop the recycling system of PV panels, especially the separation and recovery of glass from PV panels. The objective of this study was to investigate the effect of the eccentric stirring milling on the high liberation of PV panels. The typical PV panels were composed of glass, accounting for about 90 %, and ethylene vinyl acetate (EVA). During the eccentric stirring milling, glass in PV panels was selectively ground and become pieces, while EVA in PV panels was hardly ground and remained in the original coarse fraction. This was because glass was relatively brittle, while EVA was ductile. As a result, broken pieces of glass were separated from EVA, and the mutual separation and high glass recovery rate was easily achieved by the classification or sieving. The mechanism of this selective grinding of PV panel could be explained by the grinding kinetics based on a population balance model from the particle size distribution before and after grinding.

4:40 PM

(GFMAT-008-2019) Numerical investigation of a separator using water flow for efficient plastic recycling in automobile shredder residue

A. Nitta*[1]; Y. Tsunazawa[1]; S. Doi[2]; Y. Ando[3]; T. Kihara[5]; M. Harita[4]; C. Tokoro[1]

1. Waseda Univ., Japan
2. NIHON-CIM Co., Ltd, Japan
3. Kyowa Co., Ltd., Japan
4. Harita Metal Co., Ltd, Japan
5. Ecomebius Co., Ltd, Japan

In automobile recycling, plastics in automobile shredder residue (ASR) are thermally recycled because material recycling of plastics in ASR are usually financially expensive and ASR includes bromine-containing flame retardants, which is harmful to human. From the viewpoint of environmental aspects, new separation technology of plastic in ASR is strongly required. Polypropylene (PP) and polyvinyl chloride (PVC) are typical components of ASR and the difference of their specific gravity is very small. To separate PP from PVC in ASR, our group developed a new specific gravity separator using water flow. The objective of this study was to investigate the separation mechanism in the separator. We conducted numerical simulations based on discrete element method coupled with computational fluid dynamics (DEM-CFD) to clarify the separation mechanism of the separator. Simulation results showed that the separator could separate two plastics which had similar specific gravity. It was also indicated that the structure of feeder in the separator strongly affected separation behavior because plastics at relatively high feed rate clogged the feeder and reduced the separation efficiency. Therefore, it was suggested that the separator under the stable water flow and sufficient residence time could achieve mutual separation of materials with similar specific density or plastics with/without bromine.

5:00 PM

(GFMAT-009-2019) Morphological-controlled Combustion Synthesis of Aluminum Nitride Powders and Their Application

Z. Shi*[1]

1. Xi'an Jiaotong University, School of Materials Science and Engineering, China

Aluminum nitride (AlN), an important III-V group wide band-gap semiconductor, has aroused great interest due to its high thermal conductivity, good electrical resistance, low dielectric constant, and low thermal expansion coefficient, matching that of silicon. Combustion synthesis (CS) is a cost-effective method for the fabrication of aluminum nitride (AlN) powders. However, a morphology-controlled synthesis condition is still difficult to realize, which hinders the as-synthesized products for wide applications. Here, we introduce and discuss the synthesis of one-dimensional (1D) AlN nanowhiskers, 3D flower-like AlN microstructure, sphere-like AlN particles and AlN porous-shell hollow spheres with uniform morphologies by the CS process. The experimental results indicate that the morphologies of products can be controlled by manipulating the combustion parameters. Therefore, the CS of AlN with controlled grain morphologies can be achieved, which gives a chance to expand the application area of AlN ceramic. As an instance, we will show the application of the as-synthesized AlN nanowhiskers as inorganic fillers for polymer-matrix packaging materials.

G3: Crystalline Materials for Electrical, Optical and Medical Applications

Piezo/Ferro Materials

Room: Salon C
Session Chairs: Qiang Li, Tsinghua University; Danilo Suvorov, Jozef Stefan Institute

1:30 PM

(GFMAT-010-2019) The structural and dielectric properties of $Ag(Nb_{1-x}Ta_X)O_3$ (x = 0–0.8) ceramics (Invited)

D. Suvorov*[1]; L. Li[2]; M. Spreitzer[3]

1. Jozef Stefan Institute, Advanced Materials, Slovenia
2. Zhejiang U., Zijingang Campus, Department of Materials Science and Engineering, China
3. Jozef Stefan Institute, Advanced Materials, Slovenia

$Ag(Nb_{1-x}Ta_X)O_3$ (x = 0–0.8) ceramics prepared by solid-state reaction were characterized by means of their microstructure, dielectric abnormalities, polar order and MW dielectric properties. A single phase was identified using XRD for dense ceramics with x = 0–0.65, while small Ag precipitates and microstructural inhomogeneities were observed with BSE-SEM and EDS. Four kinds of dielectric abnormalities at RF frequencies were observed between −150 and 300°C. Only the peak in the ε can be observed for P1, which is due to the M2–M3 phase transition. Both the peaks in the ε and the tg δ are observable for P2 and P3, while they do not correspond to any structural phase transition. P4 exhibits a strong relaxation in the tg δ, while no abnormality in the ε can be observed. The dielectric relaxation for P4 fits well to an Arrhenius equation indicating a thermally activated process. The dielectric tunability measurement at 20–80°C reveals ferrielectricity for for x=0–0.2, antiferroelectricity for x = 0.5, and a transition behaviour for x = 0.35. Combining these results with the phase diagram, it can be concluded that the ferrielectric–antiferroelectric transition does not correspond to the M1–M2 phase transition. The MW dielectric constant for the $Ag(Nb_{1-x}Ta_X)O_3$ ceramics reaches its maximum value at x = 0.35, while the Qf value and the τ_f increase monotonously with the value of x.

2:00 PM

(GFMAT-011-2019) From common and upside-down electroceramic composites with room temperature fabrication method (Invited)

H. M. Jantunen*[1]

1. University of Oulu, Microelectronics Research Unit, Finland

Since 2014, when the first electroceramic bulks with the room temperature fabrication method was published, the progress in this field of material science has be fast. Conventional composites with dielectric and ferrite properties have been introduced showing also their feasibility to high frequency antenna structures. Here we survey these results and introduce recently invented "upside-down" electroceramic composites, which are needed when the desired electric performance can be reached if the loading level of the functional material is high enough. The procedure to fabricate the upside-down electroceramic composites at room temperature is presented and the achieved piezoelectric and ferroelectric properties are reported with a discussion on the advantages available.

2:30 PM

(GFMAT-012-2019) Polarization fatigue and domain configuration in Mn-doped Relaxor-PT ferroelectric single crystals (Invited)

Q. Li*[1]; Y. Zhou[1]; Q. Yan[1]

1. Tsinghua University, Department of Chemistry, China

Relaxor-PT ferroelectric single crystals(such as PIN-PMN-PT, etc.) with excellent dielectric, piezoelectric and ferroelectric performances are widly used as key components in actuators, sensors, transducers. Over the past decades, rare studies devoted to domain switching and polarization fatigue in novel PIN-PMN-PT and Mn-doped PIN-PMN-PT single crystals. The work are mainly focused on domain switching process in [001]-oriented rhombohedral PIN-PMN-PT and Mn-doped PIN-PMN-PT single crystals under bipolar electric field using in situ polarized light microscopy. Domain configurations in PIN-PMN-PT and Mn-doped PIN-PMN-PT crystals were confirmed by the formed domain walls. Polarization and strain loops during cyclic electric field were also studied in depth as a function of switching cycles. Polarization fatigue appeared obviously above 1000 bipolar cycles in PIN-PMN-PT samples, while Mn-doped PIN-PMN-PT samples exhibited almost fatigue-free characteristics. By considering the thermodynamic theory, the improved fatigue resistance in Mn-doped PIN-PMN-PT crystals stems from the enhancement of the barrier of domain switching. The Mn-modification would not affect the domain switching paths, but it can increase the energy barrier of domain switching, leading to the improved fatigue behaviors.

3:20 PM

(GFMAT-013-2019) Low temperature ceramic processing for sustainable ICT society (Invited)

Y. Imanaka*[1]

1. Fujitsu Laboratories Ltd., Japan

Generally, low firing process for ceramics is attractive for reducing energy consumption, resulting in low cost and low CO2 emission. Besides this generic common benefit, this process is recognized as the key technology for incorporating different materials to produce new devices in electronics ceramics field. The electronics ceramic devices such as chip capacitor, circuit board, various electronic components and modules, are always incorporated with various materials for adding different functions: ceramics for LCR and sensing function, metal for conductor and heat dissipation function, and resin for low-cost, light-weighted, and flexibility function. In other words, theses electronics ceramic devices are regarded to be the composite with different materials. Usually, the process temperature of ceramics is highest, compared with other materials like metal and resin. Therefore, the ceramic process is the bottle neck for creating new devices. The low temperature process is always expected in this field. This paper addresses basic concept of low temperature process as well as several examples of low temperature process: the multi-layered circuit board using low-temperature fireable ceramics with copper conductor, ceramic capacitor embedded organic and flexible substrate. Also, energy application such as artificial photosynthesis and the new computer architecture: digital annealer technology will be introduced.

3:50 PM

(GFMAT-014-2019) In-situ TEM visualization of graphitization process: Towards interconnection and nanosoldering applications for future nanodevices (Invited)

M. Tanemura*[1]; S. Sharma[1]; M. Araby[1]; S. Elnobi[1]; M. Rosmi[2]; Y. Yaakob[3]; G. Kalita[1]; M. Yusop[4]

1. Nagoya Institute of Technology, Department of Physical Science and Engineering, Japan
2. Universiti Pendidikan Sultan Idris, Malaysia
3. Universiti Putra Malaysia, Malaysia
4. Universiti Teknologi Malaysia, Malaysia

Graphitized nanocarbon, such as carbon nanotubes (CNTs) and graphene, is one of the key materials in nanotechnology, nanomaterials science and energy-related devices. For their practical applications, such as interconnections, their controllable growth in crystallinity (quality), size, position, temperature should be achieved. In this talk, based on the findings of the in-situ transmission electron microscopy (TEM) observations of the graphitization process, a challenge towards nanosoldering for the interconnection application and the graphene growth at lower temperatures will be dealt with. For the in-situ dynamic TEM movies, amorphous carbon nanofibers

(CNFs) including various kind of metal nanoparticles were fabricated by Ar^+ ion irradiation to carbon foil edges with a simultaneous supply of those metals. Then, the transformation process from the amorphous CNF to carbon nanotube (CNT) and to graphene nanowire induced by resistive Joule heating in TEM was observed in-situ in detail. By controlling the electromigration of the nanoparticles, such as Pt, included in CNTs, wiring and the Y-junction formation of the separated two and three CNTs by nanosoldering in TEM, respectively, were realized. In addition, thanks to the detailed TEM observation, novel catalysts enabling the graphene growth at 150ºC were demonstrated.

4:20 PM

(GFMAT-015-2019) 2D Ferroelectrics (Invited)

M. Osada*[1]

1. Nagoya University, Japan

Two-dimensional (2D) nanosheets encompassing a broad range of novel electronic, magnetic, optical and thermal properties have attracted great interests over the past decade, promising the development of next-generation multifunctional devices. Among various functionalities, ferroelectricity widely exploited for the applications in memories, capacitors, actuators, and sensors is relatively scare in 2D materials. We are working on the creation of 2D ferroelectric oxides and the exploration of their novel functionalities in electronic applications. Recently, we found room-temperature ferroelectricity in 2D perovskites ($Ca_2Na_{m-3}Nb_mO_{3m+1}$) with a non-centrosymmetric structure. In $Ca_2Na_{m-3}Nb_mO_{3m+1}$, polarizability of perovskite layers can be controlled by m, and such atomic layer engineeringexhibits the high-kdielectric response with ferroelectric instability. Switchable polarization is observed down to ~2 nm (three perovskite units). To demonstrate these 2D ferroelectricity materials, we prepared complex nanodevices and superstructured nanohybrids such as field-effect transistors and artificial multiferroic materials. The addition of ferroelectricity to the 2D materials opens up new possibilities for novel applications based on ferroelectricity.

G5: Advanced Functional Materials, Devices, and Systems for Environmental Conservation, Pollution Control and Critical Materials

Advanced Functional Materials, Devices, and Systems I

Room: Trinity III
Session Chairs: Shu Yin, IMRAM, Tohoku University;
Satoshi Wada, University of Yamanashi

1:30 PM

(GFMAT-016-2019) Modification of titanium surface environment by ECR plasma oxidation, and calcification behavior (Invited)

H. Masumoto*[1]

1. Tohoku University, Frontier Research Institute for Interdisciplinary Sciences (FRIS), Japan

Metal Ti is used by dentistry and orthopedics as an implant material, since it is excellent in biocompatibility or mechanical property. It is known that the biocompatibility of Ti will change with the environment of the surface oxide (titania: TiO_2) film of implant Ti. However, since the thermal expansion difference of Ti and TiO_2 is large, it is difficult to deposit the good TiO_2 film on Ti at low temperature for a short time. Electron cyclotron resonance (ECR) plasma is high-active plasma and highly quality crystalline films can be obtained at low temperature. On the other hand, calcium phosphate, such as hydroxyapatite, β-tricalcium phosphate and octacalcium phosphate [OCP], are utilized as the coating materials for improving the osteoconductive activity. Our previous studies indicated that implantation of OCP efficiently enhanced bone regeneration compared to HAp. In the present study, TiO_2 films were deposited on metal Ti by ECR plasma oxidation and the effect of oxidation conditions on structure and precipitation behavior of OCP were investigated. Crystalline rutile-type TiO_2 films were obtained above 300C. The amount of rutile TiO_2 increased with increasing oxidation temperature. The ECR plasma was significantly effective to prepare crystallized TiO_2 films at low temperatures. Mixtures of OCP and dicalcium phosphate dihydrate (DCPD) peaks were observed after calcification.

1:55 PM

(GFMAT-017-2019) Fabrication technique for functionally graded porous materials by use of spherical integrated granules (Invited)

H. Muto*[1]; K. Tsuzuki[1]; A. Yokoi[1]; T. W. Kian[1]; G. Kawamura[1]; A. Matsuda[1]

1. Toyohashi University of Technology, Japan

Functionally graded materials are a new emerging class of advanced materials, very attractive for an extensive range of engineering applications. The spherical integrated glanules with various compositions consisted of ceramics powder and polymer particles were prepared via electrostatic attractive integration technique. Functionally graded porous materials with the porosity ranging from 0 to 50% have benn successfully fabricated in this study.

2:20 PM

(GFMAT-018-2019) Removal of Methylene blue from Aqueous Solutions Using Activated Rice Husk Biochar: Adsorption Isotherms, Kinetics and Error analysis

F. S. Nworie*[1]

1. Ebonyi State University, Abakaliki, Industrial Chemistry, Nigeria

Removal efficiency of methylene blue (MEB) from aqueous media was studied under different experimental conditions of pH, contact time and initial concentration of the adsorbate. Activated rice husk biochar (ARHB) was characterized using BET surface area and XRD. The XRD diffraction indicated amorphous nature of the biochar with pore size (cc/g) and pore surface area (m2/g) of 9.369 and 27.32 respectively from BET surface area plot. Equilibrium isotherm based on coefficient of non- determination indicated Hills model as the best fit model while Fowler–Guggenheim model present the poorest. Based on the highest correlation coefficient and the lowest values of the error functions applied to the kinetic models, Weber and Morris intra-particle diffusion and liquid film diffusion were noted to be in control of the sorption rate. The MEB sorption capacity of the activated biochar was 356.99 mmolkg-1 which was in the range of commercially available activated carbons and other biosorbents.

2:35 PM

(GFMAT-019-2019) Ammonolysis-free synthesis strategy of metal oxynitrides and oxycyanamides (Invited)

K. Katagiri*[1]; R. Okada[1]; K. Kawanishi[1]; K. Inumaru[1]

1. Hiroshima University, Department of Applied Chemistry, Japan

Mixed-anion compounds are solid-state materials containing more than one anionic species in a single phase. They have attracted considerable attentions as novel functional materials, such as (photo) catalysts, environmentally friendly pigments, and white light-emitting diodes (LEDs). The synthesis of mixed-anion compounds containing nitrogen, i.e., oxynitrides and oxycyanamides, are generally conducted by nitridation of metal oxide precursors using gaseous NH_3. However, the use of gaseous NH_3 incurs a relatively high risk. In this study, a facile method was successfully developed to prepare metal oxynitrides and oxycyanamides. Urea was employed as a solid-state nitriding agent, instead of gaseous NH_3, to increase the safety of the reaction. Firstly, a perovskite-type metal oxynitrides, $LaTiO_2N$, has been prepared. $LaTiO_2N$ could be obtained by heat-treatment of the mixture of hydrothermally prepared $La_2Ti_2O_7$ and urea in a flow of N_2. Next, $La_2O_2CN_2$

has been successfully prepared via the cyanamidation of $La(OH)_3$ using urea. We have also prepared $La_2O_2CN_2:Eu^{3+}$, for potential application as a red phosphor. The charge transfer band of the excitation spectrum of $La_2O_2CN_2:Eu^{3+}$ was broader than that of $La_2O_3:Eu^{3+}$. This indicates that $La_2O_2CN_2:Eu^{3+}$ is efficiently excitable at the near-ultraviolet wavelength region and can be expected to be a versatile candidate as a red phosphor for white LEDs.

Advanced Functional Materials, Devices, and Systems II

Room: Trinity III
Session Chairs: Hiroshi Masumoto, Tohoku University; Hiroyuki Muto, Toyohashi University of Technology

3:20 PM

(GFMAT-020-2019) Solvothermal Synthesis and Characterization of Oxide Based Oxygen Storage Materials (Invited)

S. Yin*[1]

1. IMRAM, Tohoku University, Japan

Oxygen storage capacity (OSC) materials have potential applications in energy storage, energy transfer and automotive three-way catalysts (TWCs) etc. Ceria-based materials are well-known OSMs which already show their application as TWCs for the removal of NO_x, CO, and hydrocarbons from automobile exhaust emission. The redox property of ceria can be greatly enhanced by introduce of zirconium ions into the lattice to produce a solid solution. Compare with high temperature material synthesis process, the environmental friendly green chemical process low environmental loading, prefer to produce nanosize of particles, and also advantages to obtain the morphology controllable crystalline. In the present talk, hydrothermal and solvothermal synthesis of some OSC functional materials such as ceria based materials with Al and Sn doping, SnO_2 based materials doped with alkali earth elements, and some hexagonal ternary manganese based materials such as $YMnO_3$ etc. will be focused. The synthesis, crystalline structure, thermal stability and OSC characterization will be introduced.

3:45 PM

(GFMAT-021-2019) PM oxidation activity of metal-loaded perovskite-type oxide catalyst (Invited)

H. Yahiro*[1]

1. Ehime University, Japan

The removal of particulate matter (PM) is progressively developed as a catalytic process for the environmental protect. Up to date, silver-loaded ceria (Ag/CeO_2) has been reported to be the best catalyst for the removal of PM. However, little is known about the catalytic activity of Ag-loaded perovskite-type oxide for PM oxidation. In the present study, the catalytic activity of PM oxidation was examined for $Ag/LaFeO_3$ catalysts prepared by different methods: a conventional impregnation method with $AgNO_3$ solution on $LaFeO_3$ (Method I) and a thermal decomposition of heteronuclear cyano-complex which had adsorbed Ag ions (Method II). The PM oxidation activity over $Ag/LaFeO_3$ catalysts strongly depended on the preparation method. No or less promotive effect of Ag addition on the catalytic activity was observed for PM oxidation of perovskite-type oxide prepared by Method I. On the other hand, Method II was significantly effective for enhancing the catalytic activity of PM oxidation. It was found that the catalytic activity of $Ag/LaFeO_3$ prepared by Method II was comparable to that of Ag/CeO_2 which has been considered to be the potential candidate for PM oxidation. FE-SEM measurements demonstrated that $Ag/LaFeO_3$ prepared by Method II provided high dispersion state of Ag, compared to $Ag/LaFeO_3$ prepared by Method I.

4:10 PM

(GFMAT-022-2019) Solvothermal Synthesis of Barium Titanate Nanocubes and Their Assembly (Invited)

S. Wada*[1]

1. University of Yamanashi, Material Science and Technology, Japan

To enhance physical properties, it is known well that polarization rotation mechanism is very important for dielectric and piezoelectric materials on the basis of “interface engineering”. To apply the polarization rotation mechanism for property enhancement, a new material design using different complex oxide nanocubes was proposed. In this study, barium titanate ($BaTiO_3$, BT) nanocubes was prepared by a simple and conventional solvothermal method without surfactants or capping agents. The obtained BT nanocubes were confirmed as ones with a size of around 100 nm. Then, for a dispersion of BT-nanocubes, electric double-layer mechanism was applied and as a result, well dispersed BT nanocubes were clearly observed. Finally, the well-dispersed BT nanocubes were accumulated with sizes over 10 x 10 mm by capillary force at room temperature to measure dielectric properties. The detailed experimental procedure and dielectric properties will be reported at the conference.

4:35 PM

(GFMAT-023-2019) High oxide-ion conductivity by the overbonded channel oxygens in Si-deficient $La_{9.565}(Si_{5.826}Va_{0.174})O_{26}$ apatite without interstitial oxygens (Invited)

M. Yashima*[1]; K. Fujii[1]

1. Tokyo Institute of Technology, Japan

Apatite-type rare earth silicates are attractive materials with exhaust application such as solid-oxide fuel cells, due to its extremely high oxide-ion conductivity below 600 ºC. Interstitial (excess) oxygens have been believed to be responsible for the high conductivity in apatite-type materials. On the contrary, the present study clearly reveals the presence of Si vacancies Va in La-rich $La_{9.565}(Si_{5.826}Va_{0.174})O_{26}$ instead of the interstitial oxygens, by single-crystal neutron and X-ray diffraction analyses, density measurements and ab initio electronic calculations. Higher mobility (lower activation energy) of oxide ions along the c axis is a dominant reason for the high oxide-ion conductivity of $La_{9.565}(Si_{5.826}Va_{0.174})O_{26}$, compared with $La_{9.333}Si_6O_{26}$. The excess La cations yield the overbonded channel oxygens, leading to their highly anisotropic atomic displacements and high oxygen mobility along the c axis. The novel finding of the overbonding effect without interstitial oxygens would open new window in the design of better ion conductors. The present work has been published in Fujii, K., Yashima, M., et. al. (2018). High oxide-ion conductivity by the overbonded channel oxygens in Si-deficient $La_{9.565}(Si_{5.826}Va_{0.174})O_{26}$ apatite without interstitial oxygens.

G8: Advanced Batteries and Supercapacitors for Energy Storage Applications

Na-ion Battery

Room: Salon D
Session Chair: Palani Balaya, National University of Singapore

1:30 PM

(GFMAT-024-2019) Recent advances in Na-ion materials: From energy to power

M. Arnaiz[1]; J. Gómez-Cámer[1]; E. Gonzalo[1]; N. E. Drewett[1]; J. Ajuria[1]; E. Goikolea[2]; M. Galceran[1]; T. Rojo*[1]

1. CIC energiGUNE, Spain
2. University of the Basque Country UPV/EHU, Inorganic Chemistry, Spain

Rapid increases in Li cost and scarcity has driven research into supplementation and replacement, with Na-ion technology proving a popular alternative. In this presentation, we will explore current

state-of-the-art Na-ion batteries, including the most promising cathodes (polyanionics and $Na_xMM'O_2$ layered oxides, M, M′= Mn, Fe, Mg, Ti, etc.) and anodes (cheap hard carbon-based, as well as high energy density intermetallic and alloying materials). Recent research into nascent Na-ion hybrid capacitors (a coupled supercapacitor- and faradic-type electrode) will be considered, including remaining challenges (e.g. initial pre-metalation, safety and cost) and the promising development of low-cost hard carbon and high-performance intermetallic electrodes. For instance, a hybrid system using olive pit derived HC and activated carbon (AC) surpasses its AC/AC EDLC counterpart in terms of power density (values of up to 10 kW kg_{AM}^{-1}), while the $TiSb_2$/AC hybrid system is capable of delivering 65 Wh kg_{AM}^{-1} at 11 kW kg_{AM}^{-1} - among the best values reported for alloying materials in NICs. Finally, we will highlight future pathways for Na-ion development.

2:05 PM

(GFMAT-025-2019) Towards new silicate materials for Na-ion batteries (Invited)

A. Liivat*[1]

1. Uppsala University, Department of Chemistry - Ångström Laboratory, Sweden

The absence of low-cost positive electrode material with a sufficiently high energy-density for large-scale applications is arguably the most serious bottleneck facing us. Silicates of Fe and Mn have been studied in this context for Li-ion batteries for more than a decade. However, a leap in the sustainability of raw materials would be achieved if such silicates were enabled in Na-ion battery applications. Here an account of addressing this challenge is presented exemplifying different structure types from both modelling and experimental perspective.

2:35 PM

(GFMAT-026-2019) Elucidating structural transformations of electrodes while they are being used: The wonderful world of in situ synchrotron X-ray and neutron diffraction

N. Sharma*[1]

1. University of New South Wales, Australia

Electrodes account for a significant proportion of battery function, where atomic-scale perturbations or changes in the crystal structure during an electrochemical process permit the reversible insertion/extraction of charge carriers. A method to both understand battery function and improve their performance is to probe the crystal structure evolution operando or in situ, i.e., while an electrochemical process is occurring inside a battery. In undertaking in situ and operando experiments there are a number of critical factors that need to be considered, for example optimised cell design to marry electrochemical performance with sufficient diffraction signal. Once the practicalities of such experiments are achieved, the parameter space that can be explored and correlated allows for unprecedented insight into function. Electrochemical parameters such as applied current rates, potential cut-offs and long term cycling can be correlated to chemical parameters such as composition and particle size distribution. Using this information we can design next generation electrode materials, optimising electrochemical performance parameters at a crystallographic level. This talk will highlight our recent work on the structural evolution of $LiNi_xMn_yCo_zO_2$ and $Na_{2/3}Fe_xMn_{1-x}O_2$ families of compounds for during battery function.

Mg-ion Battery

Room: Salon D

Session Chair: Teófilo Rojo, CIC energiGUNE

3:20 PM

(GFMAT-027-2019) Defining Conduction Pathways in Cathode Materials: Resolving Logjams through Atomistic Design and Mesoscale Structuring (Invited)

S. Banerjee*[1]

1. Texas A&M University, Chemistry, USA

The deficiencies of electrochemical energy storage are a major constraint in many areas of technological design. Using a canonical intercalation host, V_2O_5, as a model system, I will discuss the structural and electronic origins of diffusion barriers in cathode materials. Scanning transmission X-ray microscopy measurements in conjunction with resonant inelastic X-ray scattering and density functional theory provide a rich picture of the evolution of electronic structure with increasing intercalation. The mitigation of diffusion impediments will be discussed with reference to the stabilization of metastable phases that provide frustrated coordination environments and enable the relatively facile diffusion of polarons. This approach has led to the discovery of several promising intercalation hosts for Mg- and Ca-ion batteries. I will focus on a tunnel-structured ζ-V_2O_5 polymorph that provides an unprecedented combination of high voltage, excellent cyclability, and good capacity and will discuss further elaboration of this concept to other polymorphs of V_2O_5. A promising advantage of switching to Mg-based batteries derives from the many reports which claim that Mg is inherently non-dendrite forming. I will address the issue of whether Mg is truly impervious to dendritic growth.

3:50 PM

(GFMAT-028-2019) Combinatorial chemistry of mg-scale advanced battery materials (Invited)

E. McCalla*[1]

1. McGill University, Chemistry, Canada

In the design of advanced battery materials it is now common place to examine pseudo-ternary and even quaternary oxides. However, such systems are never thoroughly explored, in fact, typically only 10 or so samples may be made within extremely complex systems such as Li-Mn-Ni-Co-O (of interest as positive electrodes in Li-ion batteries). Herein, a platform is presented which allows for the automated synthesis and characterization (XRD, electrochemical testing, storage experiments, and impedence spectroscopy) of hundreds of mg-scale samples a week. This system is used to screen broad composition ranges in an efficient manner for improved battery performance. Examples of the use of this platform will include cathode materials for both Li- and Na-ion batteries, as well as solid electrolytes to be used in all-solid batteries.

4:20 PM

(GFMAT-029-2019) Origin of excellent/poor reversibility of magnesium-based anodes (Invited)

M. Matsui*[1]

1. Kobe University, Department of Chemical Science and Engineering, Japan

Rechargeable magnesium battery is expected as a candidate for beyond lithium-ion batteries, because of its high volumetric energy density. The limited choice of the electrolyte solutions compatible with the magnesium metal anode hinders the development of a practical battery system. Conventional electrolyte solutions such as $MgClO_4$ in propylene carbonate, easily form a passivation layer at the surface of the magnesium metal anodes. In our group, we have been working on the bulk/surface analyses of the magnesium-based anodes: magnesium metal and intermetallics. In the present study we performed spectroscopic study for the electrochemical deposition/dissolution process of the magnesium metal, specifically focusing on the formation of passivation layer. We also introduce our recent works concerinig the magnesium-based intermetallic anode Mg_3Bi_2, which is electrohcemically reversibility in a conventional electrolyte solution, and discuss the origin of the excellent reversibility.

4:50 PM

(GFMAT-030-2019) Anion coordination and electrochemistry in magnesium battery electrolyte (Invited)

T. Mandai*[1]; K. Kanamura[2]

1. National Institute for Materials Science, Rechargeable Battery Materials Group, Japan
2. Tokyo Metropolitan University, Graduate School of Urban Environmental Sciences, Japan

Magnesium rechargeable batteries (MRBs) are one of promising classes of electric energy storage systems. The lack of electrolyte materials that support Mg2+/Mg redox activity and sufficient anodic stability is however a severe problem for practical MRB materialization. For the Mg^{2+}/Mg redox process, it is well known that the presence of chloride has a significant impact on the electrochemical activity. We have indeed achieved excellent Mg^{2+}/Mg redox by combining $Mg[TFSA]_2$ and non-Grignard magnesium monochloride in glymes, while that redox activity for the simple ethereal solutions of $Mg[TFSA]_2$ is modest. In the presentation, the Mg^{2+}/Mg activity for $Mg[TFSA]_2$-based electrolytes will be discussed with respect to the anion coordination. DFT calculations combined with Raman spectral and electrochemical analysis revealed that the coordination state of [TFSA] predominates the cathodic stability of [TFSA], consequently Mg2+/Mg redox efficiency. This finding provides significant insights for designing MRB electrolytes with reasonable Mg2+/Mg redox activity and high anodic stability. The rational design of chloride-free electrolyte materials for high voltage MRBs will also be proposed on the basis of the anion coordination.

G13: Ceramic Additive Manufacturing and Integration Technologies

Innovative Application

Room: Trinity IV

Session Chair: Soshu Kirihara, Osaka University

1:30 PM

(GFMAT-031-2019) Effect of Zr addition on the microstructure and mechanical properties of additively manufactured Cu-Cr-Zr alloys (Invited)

N. Nomura*[1]

1. Tohoku University, Graduate School of Engineering, Department of Materials Processing, Japan

Additive manufacturing has been received great attention due to both the simplification of processing and fabrication of complex geometry like combustion chamber of rocket engine which are mainly consisted of Cu-based alloys. However, Cu shows low laser absorptivity around the fiber laser wave length. In this study, we tried to fabricate Cu-Cr-Zr alloy by laser powder bed fusion process (L-PBF). The gas-atomized Cu-Cr-Zr alloy powders with different Zr content were evaluated from the point of apparent and tap densities, flowability, and laser absorptivity. Microstructure was observed by OM, SEM and TEM. Mechanical properties were evaluated by tensile test. Laser absorptivity of the powder with higher Zr content was higher than that with lower Zr content. When the builds were fabricated with the same building parameters, porosity of the builds with higher Zr content was lower than that with lower Zr. This may be related to the laser absorption difference. The higher yield strength and elongation were obtained in the builds with higher Zr content. TEM observation revealed that fine Cr precipitates were confirmed in the both builds. Effect of post treatments will be discussed.

2:00 PM

(GFMAT-032-2019) Additive Manufacturing Enabled Innovative Materials and Structures for Aerospace Applications

M. C. Halbig*[1]; M. Singh[2]

1. NASA Glenn Research Center, USA
2. Ohio Aerospace Institute, USA

New processing and fabrication methods are needed for the next generation of materials and structures used in future aerospace applications. Optimized properties, new processes, and unique designs are necessary for meeting increased requirements for high efficiencies, low emissions, lightweight, and on-demand manufacturing for part replacements. Additive manufacturing offers new capabilities for achieving benefits over conventional approaches such as tailored material properties and unique structures as well as components that are more geometrically complex, compact, multi-material, innovatively cooled, integrated, and multifunctional. A wide variety of materials including metals, ceramics, and polymers are being used in additive manufacturing to develop components for aeronautics and space applications. An overview will be provided on the efforts at NASA Glenn Research Center to apply additive manufacturing toward components for hot sections, turbine engine components, heat exchangers, acoustic panels, inlet guide vanes, electric motors, and multi-functional panels and structures.

2:20 PM

(GFMAT-033-2019) Additive Manufacturing of YSZ Ceramics by Laser Engineered Net Shaping

X. Yan[1]; Y. Chen[2]; F. Wang[1]; C. Kanger[1]; M. Sealy[1]; B. Cui*[1]

1. University of Nebraska, Lincoln, Mechanical & Materials Engineering, USA
2. Oak Ridge National Laboratory, Spallation Neutron Source, USA

Compared to metals, laser additive manufacturing of ceramic materials is more challenging because of the intrinsic brittleness of ceramics and the high temperature gradients, which can induce significant defects and cracking. This presentation shows our novel research on the successful additive manufacturing of yttria-stabilized zirconia (YSZ) ceramics by a laser engineered net shaping (LENS) process. The microstructure formation, such as phase composition, grain size, and crack density, has been carefully characterized by neutron diffraction and electron microscopy, which are correlated with the LENS conditions such as the laser power. Phase transformation from monoclinic to tetragonal/cubic occurred during the LENS of YSZ ceramics. The crack density inside the manufactured parts was reduced at a higher laser power.

2:40 PM

(GFMAT-034-2019) Fabrication of Micro Photonic Crystals by Ultraviolet Laser Lithography

S. Kirihara*[1]

1. Osaka University, Joining and Welding Research Institute, Japan

Three-dimensional (3D) micro photonic crystals with a diamond structure composed of titania micro lattices were fabricated using ultraviolet laser lithography, and the bandgap properties in the terahertz (THz) electromagnetic-wave frequency region were investigated. An acrylic resin paste with titania fine particle dispersions was used as the raw material for additive manufacturing. By scanning a spread paste surface with an ultraviolet laser beam, two-dimensional solid patterns were dewaxed and sintered. Subsequently, 3D structures with a relative density of 97% were created via layer lamination and joining. A titania diamond lattice with a lattice constant density of 240 μm was obtained. The properties of the electromagnetic wave were measured using a THz time-domain spectrometer. In the transmission spectra for the Γ-X <100> direction, a forbidden band was observed from 0.26 THz to 0.44 THz. The frequency range of the bandgap agreed well with calculated results obtained using the plane–wave expansion method. Additionally, results of a simulation via transmission-line modeling indicated that a localized mode can be obtained by introducing a plane defect between twinned diamond lattice structures.

Integrated Approach

Room: Trinity IV
Session Chair: Michael Halbig, NASA Glenn Research Center

3:20 PM

(GFMAT-035-2019) Additive Manufacturing of Ceramics: Issues and Challenges (Invited)

T. Ohji*[1]

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

For realizing complex-shaped products with reduced lead-time, additive manufacturing (AM) technologies for ceramics products have been developed in “High-Value Added Ceramic Products Manufacturing Technologies” project sponsored by the Japanese government. The project deals with two technologies for producing ceramic green bodies; powder layer manufacturing (indirect selective laser sintering) and slurry layer manufacturing (stereolithography), in addition to ceramic laser sintering (direct selective laser sintering). The paper will describe the research achievements in this project, including the unique-structured 3D bodies never attainable in conventional methods. Particularly the paper addresses a number the technical items which should be carefully considered and properly selected, for optimizing the AM procedures. Issues to be solved for applying AM into actual industries will be also discussed. This work was conducted as a part of “High-value added ceramic products manufacturing technologies project” supported by CSTI, SIP, “Innovative design/manufacturing technologies (managed by NEDO)”.

3:40 PM

(GFMAT-036-2019) Functionally Graded Additive Manufacturing of Ceramics (Invited)

H. Yun*[1]

1. Korea Institute of Materials Science, Republic of Korea

Functionally graded materials (FGM) is normally defined as the structure which have the variation in composition and/or structure gradually over volume, resulting in corresponding changes in the properties of the material. Because additive manufacturing (AM) technology have a potential for controlling not only 3 dimensional (3D) structure but also the composition simultaneously, AM has recently attracted attention as the most powerful and new method of manufacturing FGM. Functionally graded additive manufacturing (FGAM) is defined as a single AM process that either uses the gradational missing of materials or controlling the density of a material to fabricate 3D freeform geometries with variable-properties within one component. Our group has developed a novel digital light process (DLP) based system, which has been designed specifically to overcome the complications of typical vat-type DLP system that use ceramic suspension. Our new system consists of multi-film type material feeding system with a 180°-horizontally rotatable stereolithography module and unique washing module to prevent contamination between materials, for structures with multi-ceramic distribution. 3D structure of alumina and zirconia with various kinds of composition gradation was successfully manufactured by using this system.

Young Professionals Forum - Next Generation Materials for Multifunctional Applications and Sustainable Development, and Concurrent Societal Challenges in the New Millennium

Advances in Biomedical Science and Engineering I

Room: Trinity I
Session Chairs: Eva Hemmer, University of Ottawa; Andy Nieto, Naval Postgraduate School

1:30 PM

(YPF-001-2019) Advanced Bioceramics – From Transparent Alumina to Graphene Nanocomposites (Invited)

A. Nieto*[1]; Y. Han[2]; J. Shackelford[3]; R. Gao[2]; K. Hwang[4]; F. Chen[2]; S. Kim[5]

1. Naval Postgraduate School, Dept. of Mechanical and Aerospace Engineering, USA
2. Wuhan University of Technology, China
3. University of California, Davis, USA
4. Gyeongsang National University, Engineering Research Institute, Republic of Korea
5. Yeungnam University, School of Materials Science and Engineering, Republic of Korea

This talk will provide an overview of recent advances in bioceramics that have been enabled by rapid ceramic processing technologies such as spark plasma sintering (SPS). In particular, the synthesis of transparent alumina and its potential applications will be discussed. SPS has enabled the sintering of dense nanograined alumina, which endows it with optical transparency. SPS has also contributed significantly to the advent of carbon nanoparticle reinforced ceramics. Carbon nanotube (CNT) and graphene nanoplatelet (GNP) reinforced ceramics have shown great promise for overcoming the low fracture toughness hurdle for many bioceramics. These reinforcements bring about exciting properties such as damage tolerance, enhanced conductivity, and reduced grain growth. GNPs are particularly exciting as reinforcements since graphene has been shown to have much better biocompatibility as compared to CNTs. A brief discussion on other prospective nanoparticle reinforcements is provided to provide direction to future research.

2:00 PM

(YPF-002-2019) Long-lifetime luminescent nanoparticles and deep-tissue imaging: From autofluorescence removal to multiplexed sensing (Invited)

E. Martín Rodríguez*[1]; D. H. Ortgies[2]; G. López Peña[1]; E. Ximendes[2]; B. del Rosal[3]; N. Fernandez[4]; D. Jaque[4]

1. Universidad Autónoma de Madrid, Física Aplicada, Spain
2. Instituto Ramón y Cajal de Investigación Sanitaria IRYCIS, Spain
3. Swinburne University of Technology, Australia
4. Universidad Autónoma de Madrid, Spain

In vivo fluorescence imaging has recently come into reality thanks to the development of new fluorophores that present emissions in the spectral regions known as biological windows, where light can penetrate deeper into biological tissue. The second biological window (1000 - 1350 nm wavelength) is gaining interest because light penetration higher than 1 cm can be obtained. However, the existence of autofluorescence in this region associated with pigmentation and diet limits the useful wavelengths to 1200 - 1350 nm. In this work, we present the elimination of autofluorescence signals in in vivo imaging, taking advantage of the long luminescent lifetimes of nanoparticles doped with trivalent rare earth ions (~100 μs) compared with the lifetime of biomolecules causing autofluorescence (<<1 ns). The combination of the large lifetimes of the former

with their emissions in the second biological window has allowed us to obtain deep tissue autofluorescence free images by using a simple time-gated set up. We will also present how the simultaneous use of nanoparticles with different luminescent lifetimes has allowed us to perform multiplexed imaging in vivo.

2:30 PM

(YPF-003-2019) Innovations in biosensor platforms toward point-of-care molecular diagnostics

S. S. Mahshid*[1]

1. Sunnybrook Research Institute, Biological Sciences Platform, Canada

Development of rapid biosensors capable of real-time monitoring of analytes in complex matrices requires innovations from combinations science and engineering, and can in principle, impact many applications including medical diagnostics, prognostics, and therapeutics. Over the past two decades, many approaches for detection of biomarkers have been explored among which, electrochemical sensors have shown a lot of promises since they are known to be rapid, reagent-less and easily multiplexed. However, given the fact that signal originates from the electron transfer, further steps need to be taken toward a specific and sensitive signal response aiming for a point-of-care biosensor platform. By engineering the sensor's surface, we demonstrate modifications such as (1) immobilization of synthetic bio-layers on the sensing electrode to provide the desired specificity in real biological samples, and (2) introducing of surface nanoroughness and microscale electrodes to provide direct analysis of clinical samples with appropriate target detection limits, and low levels of false negatives and false positives. These innovations in biosensor platforms with the help of synthetic biology and nanotechnology approaches provide multiplexing detection of proteins and small molecules at their therapeutic ranges for applications in disease diagnostics, and therapeutic monitoring.

Advances in Energy Research

Room: Trinity I
Session Chairs: Yosuke Goto, Tokyo Metropolitan University; Sankha Banerjee, California State University, Fresno

3:20 PM

(YPF-004-2019) Liquid-phase chemistry of sulfide electrolytes for all-solid-state lithium battery (Invited)

A. Miura*[1]; N. Rosero-Navarro[1]; K. Tadanaga[2]

1. Hokkaido University, Engineering, Japan
2. Hokkaido University, Japan

Sulfide electrolytes are importeant materials for all-solid-state lithium batteries because of thier high Li ion conductivity. Moreover, they aredeformable, to connect the Li ion path between grains. However, their synthesis reaction should be performed to handle sulfur species, which are moisture-sensitive and have high vapor pressures. Here, we introduce liquid-phase chemistry for the preparation of sulfide-based solid electrolytes and their application in an all-solid-state lithium battery. We introduce two liquid-phase routes of sulfide-based solid electrolytes. The first involves suspension synthesis of solid electrolytes, such as $Li_7P_3S_{11}$ via the formation of their complexes. The second is the dissolution-precipitation of sulfide-based electrolytes using a solvent with high solubility. This reaction involves precipitation from a homogeneous solution to form electrolyte layers of Li_6PS_5Cl.

3:50 PM

(YPF-005-2019) Photonic power converters and photovoltaics: Designs and materials for very high efficiencies (Invited)

K. Hinzer*[1]

1. University of Ottawa, Canada

Multijunction solar cells have demonstrated the highest solar photovoltaic conversion efficiencies presently available, reaching 46%. The multi-junction approach can be adapted for the highly-efficient conversion of monochromatic photonic power to electrical power, and conversion efficiencies of >65% have been realized. For these photonic power converters, monolithic epitaxially-grown vertically-stacked GaAs pn junctions optimally harvest light near the current-balanced wavelength, realizing an output voltage proportional to a multiple of the photon voltage (up to 24 V), while a corresponding current decrease reduces resistive losses. Applications of these devices include power-over-fiber and optically-isolated DC-DC converters. A similar structural approach can be applied to solar cells, wherein each subcell is divided into 2 or more pn junctions of carefully chosen thicknesses. Depending on the desired application and cost rationale, the need for low cost high efficiency devices is required in order to deploy high energy density photovoltaic panels. For first order efficiency increases, one may use strained quantum wells or quantum dot nanostructures in the devices to tune the absorption band gap of subcells. For further increases for low cost devices, materials such as silicon and SiGeSn must be included in the multijunction stack to replace the higher cost substrates.

4:20 PM

(YPF-007-2019) Carbon Dots: A versatile material for solar energy harvesting devices

D. Benetti*[1]; H. Zhao[3]; A. Vomiero[4]; F. Rosei[2]

1. Institut National de la Recherche Scientifique, Énergie Matériaux Télécommunications, Canada
2. INRS, Canada
3. Qingdao University, College of Physics, China
4. Lulea University of Technology, Engineering Sciences & Mathematics, Sweden

Generating power directly from solar radiation represents a promising opportunity towards addressing the increasing demand for clean energy, also reducing environmental impact caused by excessive carbon emissions. The commonly used quantum dots (QDs) for photovoltaivc applications contain toxic elements such as Pb, Cd or they require complicated synthesis methods. Very recently Carbon dots (Cdots) have gather attention as potential competitors to conventional semiconductor QDs. In fact, Cdots are exclusively composed of non-toxic elements (C, N and O) and can be synthesized in large quantities via a simple solvothermal approach. Compared to conventional semiconducting QDs, Cdots have superior advantages of non-toxicity, environmental friendliness, low-cost and simple preparation using abundant carbon based feedstock. Exploiting the ability to tune the optical and electrical properties of Cdots by changing the synthetic methods, different type of Cdots with absorption and emission spectra in visibile/Near infra red range are prepared. The charge transfer dynamics of heterostructures formed by Cdots and other different materiasl, such as TiO_2 and Graphene Oxide, is monitored by photoluminescence (PL), transient PL decays and transient photovoltage (TPV) decays. The as-prepared Cdots are then employed to realize different devices such as efficient charge transport layers for Perovskite Solar Cells and as metal-free large-area Luminescent Solar Concentrators (LSCs) with good efficiency and excellent photostability.

Tuesday, July 23, 2019

G1: Powder Processing Innovation and Technologies for Advanced Materials and Sustainable Development

Nanostructure and Microstructure Control

Room: Trinity II
Session Chairs: Hua-Tay Lin, Guangdong University of Technology; Norifumi Isu, LIXIL Corp.

8:30 AM

(GFMAT-037-2019) Preparation and properties of aluminum magnesium boride ceramics (Invited)

J. Zhang*[1]

1. Shanghai Institute of Ceramics, Chinese Academy of Sciences, China

$AlMgB_{14}$ exhibited a combination of excellent properties, such as extreme hardness, good electrical conductivity, high thermal stability, excellent wear resistance and low density, is a promising candidate for potential technical applications as cutting materials etc. In literature, several synthesis routes for processing of $AlMgB_{14}$ ceramics have been reported, however, it is still a challenge for the preparation of AlMgB14 because the synthesis route are still not well optimized. In this work, $AlMgB_{14}$ power was prepared using different precursors as reactants at high temperature. The powder properties including the phase, composition, impurities were investigated. Subsequently, the powder was densified using hot pressing. The microstructure and mechanical properties including hardness, strength and indentation fracture resistance were measured. The mechanical properties of $AlMgB_{14}$ ceramics were investigated and related to the microstructure characteristics.

9:00 AM

(GFMAT-038-2019) Lithium metal protection layer for high performance lithium metal batteries (Invited)

S. Sun[1]; U. Paik[1]; T. Song*[1]

1. Hanyang University, Department of Energy Engineering, Republic of Korea

Metallic lithium (Li) has received significant attention as a promising anode material due to the advantages of its light weight (0.53 g cm^{-3}), high specific theoretical capacity (3860 mAh g^{-1}) and the lowest electrochemical potential (-3.04V vs the standard hydrogen electrode). However, its practical use has been limited due to the dendritic Li growth, irreversible morphological change and low Coulombic efficiency during cycling. Various approaches have been suggested; i) Mechanical suppression of dendritic lithium growth. ii) Regulating Li deposition. iii) SEI layer reinforcement iv) Composite electrode engineering. Especially, the studies have been focused on the formation of Li protection layer for the control of Li ion flux and the increase of Sand's time. Here, we present the structures and composition of the lithium metal protection layer to improve the electrochemical properties. The mechanical property, electronic conductivity and ionic conductivity have been considered for the design of Li metal protection layer. The designed protection layers effectively retard the growth of dendritic lithium metal due to its better Li ion flux and the suppression of the repeated electrolyte decomposition during cycling.

9:30 AM

(GFMAT-039-2019) Densification, microstructural tailoring and performance of $Ta_{0.8}Hf_{0.2}C$-based ultra-high temperature ceramic composites

J. Yin*[1]; B. Zhang[1]; X. Liu[1]; Z. Huang[1]

1. Shanghai Institute of Ceramics, China

$Ta_{0.8}Hf_{0.2}C$ is a novel member among ultra-high temperature ceramic (UHTC) families. $Ta_{0.8}Hf_{0.2}C$-27vol%SiC (99.0% in relative density) was toughened and strengthened via pressurelessly in-situ reactive sintering process. HfC and β-SiC particles were formed after reaction of $HfSi_2$ and carbon black at 1650°C. $Ta_{0.8}Hf_{0.2}C$ was obtained from solid solutioning of HfC and commercial TaC. The β→α phase transformation of SiC proceeded below 2200°C. High aspect ratio, platelet-like α-SiC grains formed and interconnected as interlocking structures. Toughness and flexural strength values of 5.4±1.2 $MPam^{1/2}$ and 443±22 MPa were measured respectively. The toughening mechanisms by highly directional growth of discontinuous α-SiC grains were crack branching, bridging and deflection behaviors.

Low-cost and Energy-saving Processing of Advanced Ceramics and Ceramic Composites, including Smart Recycling of Materials for Sustainable Development

Room: Trinity II
Session Chairs: Rainer Gadow, Institute for Manufacturing Technologies of Ceramic Components and Composites, University of Stuttgart; Motoyuki Iijima, Yokohama National University

10:20 AM

(GFMAT-040-2019) Simple process for direct formation of photocatalytic anatase-TiO_2 on titanium-metal (Invited)

T. Ishikawa*[1]; K. Tsujikura[1]

1. Tokyo University of Science, Yamaguchi (Sanyo-Onoda City University), Japan

Titanium has emerged as being the most popular metal for bio- and environmental applications, due to its good corrosion resistance, good mechanical properties, good bio-compatibility, and light weight. Of these properties, the good corrosion resistance is coursed by existence of a passive film which consists of thermodynamically stable rutile-TiO_2. Accordingly, direct oxidations of titanium-metal only lead to formation of rutile-TiO_2 in entire temperature region. Here we report a simple process for direct formation of photocatalytic anatase-TiO_2 on titanium-metal by simple oxidation. In our process, at the first step, titanium was treated by a reduction agent to create a surface titanium hydride layer, which is thermodynamically stable compared to pure titanium; rutile-formation is effectively prevented by the existence of the abovementioned titanium hydride at room temperature. After that, the treated titanium covered with titanium hydride was immerged in an aqueous silica; subsequent calcination effectively generated the surface anatase layer. It's because the covered silica stabilized the formed anatase phase; at the interface between TiO_2 and SiO_2, atoms constructing TiO_2 are substituted into the tetrahedral silica lattice, forming tetrahedral Ti sites. In this paper, the photocatalytic activity of the obtained titanium covered with anatase TiO_2 will be described.

10:50 AM

(GFMAT-041-2019) The comparison between mechanochemical process by planetary ball milling and heating process for crystal structure change of cerium and yttrium minerals in weathered residual rare earth ores

T. Kato*[1]; C. Tokoro[2]

1. Waseda University, Graduate School of Creative Science and Engineering, Japan
2. Waseda University, Japan

The objective of this study is to compare between mechanochemical process by planetary ball milling and heating process for crystal structure change of cerium and yttrium minerals in weathered residual rare earth ores from the point of view of power consumption. For this purpose, the weathered residual rare earth ores were ground by planetary ball mill without and with solid sodium hydroxide and heated by microwave reactor. After these processes, the samples were investigated by x-ray absorption fine structure (XAFS) in cerium L_{III} and K-edge and yttrium K-edge to confirm the effect on the crystal structure of the cerium and yttrium minerals and phase composition of the ores by planetary ball milling and heating. From above experimental results, it was revealed that a part of tetravalent cerium in cerium minerals was reduced to trivalent cerium by both planetary ball milling without solid sodium hydroxide and heating. In addition, the yttrium minerals was changed to yttrium hydroxide by both planetary ball milling with solid sodium hydroxide and heating. On the point of view of power consumption, it was confirmed that mechanochemical process was more economical than heating process to acheive crystal structure change of cerium and yttrium minerals.

11:10 AM

(GFMAT-042-2019) Characterization of milled carbon fiber as filler powder for composite materials

D. Shimamoto*[1]; Y. Sugimoto[1]; Y. Hotta[1]

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

Recently, carbon fiber reinforced plastic is a material expected to be used as a lightweight structural material. On the other hand, in order to use carbon fiber reinforced plastics, it is necessary to be strongly aware of circular economies including collection and recycling. By repeating collection and recycling, it is known that the form of carbon fiber as reinforcing fiber changes from fiber to milled powder. In this study, we studied the characterization of milled carbon fiber as filler powder for composite materials.

11:30 AM

(GFMAT-043-2019) High Quality Advanced Materials Designed by Smart Powder Processing

M. Naito*[1]; T. Kozawa[2]; A. Kondo[2]

1. JWRI, Osaka University, Japan
2. Osaka University, Joining and Welding Research Institute, Japan

Smart powder processing stands for green and sustainable powder processing technique that creates advanced materials with minimal energy consumption and environmental impacts. Particle bonding technology is a typical smart powder processing technique to make advanced composites. It creates direct bonding between particles without any heat support or binders of any kind in the dry phase. The bonding is achieved through the enhanced particle surface activation induced by mechanical energy. By using this method, one-pot processing achieving both the synthesis of nanoparticles and their bonding with another kind of particles to make nanocomposite granules was developed. In this talk, applications of this processing for low temperature mechanical synthesis of LED materials such as YAG phosphor and the one-pot mechanical synthesis of cathode materials for lithium ion batteries will be explained.

Advanced Powder Processing

Room: Trinity II
Session Chair: Junichi Tatami, Yokohama National University

1:30 PM

(GFMAT-044-2019) From Flash Sintering to Electric Field Effects on Microstructural Evolution: ZnO as an Example (Invited)

J. Nie[1]; C. Hu[1]; J. Luo*[1]

1. University of California, San Diego, USA

This talk will first review a series of our studies of flash sintering using ZnO as a model system. A coupled thermal and electric runaway model has been developed to forecast the onset flash temperatures [Acta Mater. 94:87 (2015)]. Further studies suggested that the rapid heating profiles enable the ultrafast densification rates [Acta Mater. 125:465 (2017)]. A two-step flash sintering (TSFS) technology was invented to densify nanocrystalline ceramics with suppressed grain growth [Scripta Mater. 141: 6 (2017)]. In a new water-assisted flash sintering (WAFS) technology, we can start a flash at room temperature to subsequently densify a ZnO specimen to ~98% densities in 30 s (without any furnace heating!) [Scripta Mater. 142: 79 (2018)]. The relevant scientific questions and technological opportunities of flash sintering are discussed in a recent Viewpoint Article [Scripta Mater. 146: 260 (2018)] Moreover, recent (unpublished) results on the effects of Bi_2O_3 vs. Al_2O_3 doping on the flash sintering of ZnO will be presented. Subsequently, most recent on-going studies of the electric field effects on microstructural developments in Bi_2O_3-doped ZnO, including results from controlled grain growth experiments, along with coupled aberration-corrected STEM characterization and DFT modeling of an underlying grain boundray structural (complexion) transition, will also be discussed in detail.

2:00 PM

(GFMAT-045-2019) Control on Density of Highly Textured $Ca_3Co_4O_9$ Ceramics Using a Hot-Forging Sintering for Efficient Thermoelectric Applications

R. Shimonishi*[1]; M. Hagiwara[2]; S. Fujihara[1]

1. Keio University, Japan
2. Keio University, Department of Applied Chemistry, Japan

$Ca_3Co_4O_9$ (CCO) is regarded as an alternative to heavy-metal-based thermoelectric materials. Recently, porous CCO ceramics with a relative density of 65% and a Lotgering factor f of 0.21 have been reported to exhibit a superior thermoelectric performance. In this work, we have fabricated density-controlled CCO ceramics with higher f values by a topotactic solid-state reaction. $CaCO_3$ powder was added to a $Co(OH)_2$ solution synthesized by a homogeneous precipitation method. The mixed powder was uniaxially pressed into pellets under a pressure of 300 MPa and then converted into a single phase of CCO by a hot-forging sintering at 900 °C for 1 h under a pressure from 0 to 5 MPa. The resulting CCO ceramics were highly oriented with a f value of about 0.9 for the (00l) planes. In SEM observation, the CCO plate-like particles ca. 130 nm in thickness were stacked to form slit-like pores between the CCO particles. It is assumed that phonon with long mean free path is scattered to decrease thermal conductivity. By increasing the pressure in hot-forging sintering, the relative density of CCO ceramics could be increased from 41% to 84%. Furthermore, the lower density samples also exhibited the high orientation. As a result, the electrical conductivity was higher than that of the previous ceramics with the similarly lower density.

2:20 PM

(GFMAT-046-2019) Preparation of solid sliding composite by non-sintering solidification process

R. Nojiri*[1]; H. Razavi Khosroshahi[1]; M. Fuji[1]

1. Nagoya Institute of Technology, Japan

Emission of green house gases such as carbon dioxide has become a serious environmental issue in recent decades. Fabrication of ceramic materials, which usually requires a firing process at high temperatures, generates a huge amount of green house gases. To develop an eco-friendly process for ceramics manufacturing, elimination of firing process from ceramics production is necessary. In our research group, we propose a solution for this problem via a chemical solidification of inorganic powder using mechanochemical surface activation. In this method, a solid with mechanical properties comparable to sintered ceramics from inorganic powders is obtained at room temperature. Ceramics produced through this method are called "Non-firing ceramics". Non-firing process will be able to fabricate new conceptual composite and hybrid materials, because the process takes place at room temperature. In this presentation, I will introduce you to fabricate solid sliding composite through non-sintering solidification process.

Advanced Characterization and Analytical Techniques for Powder Processing and Materials

Room: Trinity II
Session Chair: Junichi Tatami, Yokohama National University

3:20 PM

(GFMAT-047-2019) Biomimic Anti-stain Surface Treatment for Housing Wet Area (Invited)

N. Isu*[1]

1. LIXIL Corp., Material and Property Analysis Laboratory, Japan

The fundamental way of thinking on the human and the earth conscious manufacturing and examples were discussed. One of the biggest suffering at home is a cleaning around the wet area where water is used. Much energy and resources are consumed for eliminating dirt or stain at home as well as buildings. Anti-stain surface treatments mimicking snail shell are applied to housing wet area resulting in the decrease of the housekeeping energy. In this paper, ceramic tile and sanitary ware are reported. The shell of snail is always clean on rainy days. Because many small grooves on the surface of the shell play a role like a rain gutter, the water film forms on the shell surface to prevent oily dirt. The dirt easily comes off with a little rain. Although ceramic tiles are originally hard to get dirty, it is necessary to be more hydrophilic than ordinary tiles for urban dirt including oil content like smoke. By coating with higher hydrophilic nanoparticles on ceramic tile, the oil containing dirt is easily removed with rain alone. The antibacterial treatment is necessary to keep hygiene environment around wet area. Ag is applied to the sanitary ware glaze as an antibacterial agent. The glaze is amorphous aluminosilicate with 0.08 wt% Ag. The XAFS spectrum of Ag-glaze were quite similar to that of $AgNO_3$ aqueous solution. This indicates that silver exist as monovalent cation in the glaze without forming crystal structure.

3:50 PM

(GFMAT-048-2019) Investigation of Cr(III) substituted spinel type mixed oxide as catalytic materials for water oxidation

T. Kanazawa*[1]; S. Nozawa[2]; K. Maeda[3]

1. Tokyo Institute of Technology, Chemistry, Japan
2. Institute of Materials Structure Science, Japan
3. Tokyo Institute of Technology, Japan

Water oxidation to produce O_2 (OER; oxygen evolution reaction), which is anodic side of water splitting, is a difficult reaction because 4 electrons are required. Previously, we synthesized $Fe_{2-x}Cr_xO_3$ oxide particle as a catalyst for water oxidation. From the result, Cr (III) was revealed as an effective element to enhance OER activity. However, the catalytic performance of $Fe_{2-x}Cr_xO_3$ is not satisfactory, due primarily to the anodic dissolution of the Cr(III) component that may arise from the host Fe_2O_3 framework. In this work, we focus Al and Cr based spinel oxide; $MAl_{2-x}Cr_xO_4$ (M: Ni, Cu, Co). Many spinel type oxides were reported as efficient water oxidation catalysts. In addition, spinel oxides consist of two cations with different charges: A^{2+} and B^{3+}. With this compositional flexibility, Cr(III)-substitution as well as improved performance for water oxidation is expected. The OER activities of C(III)-substituted spinel oxides were investigated by means of electrochemical and photochemical measurements. Photochemical reaction was evaluated under visible light irradiation ($480 < \lambda < 500$ nm) in the presence of tris(2,2′-bipyridyl)ruthenium(II) sulfate and sodium persulfate. Electrochemical measurement was conducted in a phosphate buffered aqueous solution (pH 7.5) using $MAl_{2-x}Cr_xO_4$ particles, which were loaded on a FTO electrode, in the presence of an electrochemical bias. The results indicated that Cr(III)-substituted $CoAl_2O_4$ is a good candidate as an OER catalyst.

4:10 PM

(GFMAT-049-2019) ZrN:(Eu/La) nano-particles through carbothermal nitridation

G. Westin*[1]

1. Uppsala University, Sweden

Zirconium nitride ceramics are used, or considered for a wide range of applications including, optical, solar hydrogen catalysis, electrical storage, and as matrix for nuclear fuels where La simulates Ac and Am waste to be burnt. Often nano-particles are required for these applications, either for their large surface area in devices, or as starting powders for sintering into high density compacts, for use as nuclear fuels. In this work, carbothermal nitridation of Zr-carbon- or La/Eu/Zr-carbon gels to un-doped or La/Eu-doped ZrN nano-phase powders is presented. Traditional powder based carbothermal processes achieve poor mixing of the constituent compounds which results in high synthesis temperatures and long annealing times, yielding large and extensively agglomerated powders. A solution based method using sucrose-Zr-La-alkoxide and sucrose-Zr-Eu-alkoxide as precursors is described in detail, using TG-DT analysis, XRD, IR- and Raman spectroscopy, XPS, SEM-EDS, TEM-EDS. It was found that the phase evolution differed when the redox stable La^{3+} was used compared to the redox active Eu^{3+}, where the latter formed $EuZrO_3$ and the former $La_2Zr_2O_7$ as intermediate phases. Both doped systems ended with cubic Ln-doped ZrN at 1495°C, which could also contain some O and or C, mixed with carbon.

4:30 PM

(GFMAT-050-2019) In-situ observation of internal strucutre of ceramic slurry, green body and sintered body by optical coherence tomography

J. Tatami*[1]; T. Takahashi[2]; M. Iijima[3]

1. Yokohama National University, Japan
2. Kanagawa Institute of Industrial Science and Technology, Japan
3. Yokohama National University, Graduate School of Environment and Information Sciences, Japan

Properties of ceramics strongly depend on their internal structure, which is drastically changed during the powder processing. Optical coherence tomography (OCT) is the novel technique to be able to obtain the image of the internal structure of opaque materials rapidly and 3-dimensionally, which has been developed in the field of medical application. In this study, the OCT was applied to observe internal structure of ceramic slurry, green and sintered bodies. Brownian motion of Si_3N_4 particles in the slurry and anisotopic drying of the slurry were observed in real-time. Internal structure of the green body prepared by dry pressing resulted from the used granules. Artificially induced pores and cracks in the Al_2O_3 sintered body were clearly found by OCT observation. OCT observation of the green body was also carried out during firing. As a result, shrinkage and chenge in the internal strucure during sintering were successfully observed eve at high temperatures. Consequently, it was shown that the OCT observation is useful to understand the change in the internal strucutre of ceramics during powder processing.

G2: Novel, Green, and Strategic Processing and Manufacturing Technologies

Novel, Green, and Strategic Processing I

Room: Trinity IV

Session Chairs: Tatsuki Ohji, National Institute of Advanced Industrial Science and Technology (AIST); Surojit Gupta, University of North Dakota

1:30 PM

(GFMAT-051-2019) Sustainability, Diversity and Inclusion in a Global Landscape: Implications in the field of Material Sciences research (Invited)

L. Birla*[1]

1. Elsevier, Materials Sciences, Netherlands

Elsevier's report on Sustainability Science in a Global Landscape, in collaboration with SciDev.Net, contributes to the understanding of sustainability science as a research field and facilitates the dialogue between science and society in sustainable development. In this relatively young field, the study establishes a baseline, both in the definition and the understanding of sustainability science, from which we may follow its progression and trajectory. Six key themes that encompass the United Nations Sustainability Development Goals are examined in the report: Dignity, People, Prosperity, Planet, Justice and Partnership. Adding to this study in-house analytic expertise (SciVal, Scopus and Research Intelligence) an overview on sustainability, as well as diversity and inclusion in material sciences is given. Trends over the past decade will be presented and evaluated, identifying future developments conducive to a more inclusive, diverse and sustainable future of research.

2:00 PM

(GFMAT-052-2019) Eco-Materials Processing and Life Cycle Assessment (Invited)

Z. Nie*[1]

1. Beijing University of Technology, College of Materials Science and Engineering, China

In this presentation, a brief review of the recent advances in the field of Eco-materials were performed, giving opinions on the current activities and suggesting possible future courses of action, and a review of recent developments of LCA methodology and applications in China were offered also. As the abbreviation of environmental conscious materials or ecological material, Eco-materials was focused to solve the problem that the traditional research and development of materials aim on the improvement of service performance but often neglect the large amount of energy consumption and pollution emission caused by materials production and related stages (e.g. mining, transportation and so on). The concept of Eco-materials suggests that the development of materials should not only consider the service performance, but also try best to decrease the environmental impact during the whole life cycle, and had been widely accepted by society and materials industry in recent year. The identification and reduction of processing environmental load, resource optimization and design of renewable materials is the main prospects of the environment-friendly technology development of engineering materials. LCA (life cycle assessment) is an effective tool to enable the decision-making and technical support to the target of energy-saving and emission-reducing. The life-cycle big data platform established in BJUT is to be introduced.

2:30 PM

(GFMAT-053-2019) Monoethanolamine for Rare Earth Recovery (Invited)

P. Kim*[1]; G. Das[2]; M. Lencka[2]; A. Anderko[2]; R. Riman[1]

1. Rutgers University, Materials Science and Engineering, USA
2. OLI Systems, Inc., USA

Increasing global demand for rare earth elements (REE) necessitates improved or new methods of chemical processing for sustainable and economical rare earth isolation and purification. Current refinement processes utilize large quantities of chemicals such as HCl, $(NH_4)_2C_2O_4$, and NaOH, which present unique technical and environmental problems. This presentation will demonstrate the use of thermodynamic process simulations to establish a new method of REE recovery from aqueous solutions at industrially relevant conditions. Simulations of the monoethanolamine (MEA) – H_2O – REE chloride – CO_2 ternary system identified conditions at which the full recovery of aqueous REEs from solutions at concentrations ranging from 100 to 56000 ppm as carbonate solids is possible. Experimental results support these predictions as > 99% of aqueous REEs were recovered as their respective normal carbonate solids. These findings suggest that this technology with the aid of thermodynamic simulations may be used to effect high yield REE recovery from more complex aqueous environments.

3:20 PM

(GFMAT-054-2019) Current Progress in the Design of Novel Green Materials by Using Lignin as a Feedstock

S. Gupta*[1]

1. University of North Dakota, Mechanical Engineering, USA

There is an urgent need for designing green materials which can reduce Carbon foot print. In this presentation, I will present some of the recent studies in my research group on the design of novel lignin based materials. For example, I will present research on recent developments in two main areas: (A) green polymeric composites, and (B) carbonaceous porous materialsby using lignin as feedstock. It is expected that these novel materials can be used for multifunctional applications.

3:40 PM

(GFMAT-055-2019) Spontaneous Coagulation Casting: Invention and development

X. Mao*[1]

1. Shanghai Institute of Ceramics, Chinese Academy of Sciences, China

Spontaneous coagulation casting is a novel ceramic shaping method developed by Shanghai Institute of Ceramics in past decade. The modified alternating copolymer of isobutylene and maleic acid is used as an additive for ceramic slurry. After casting, the flowable slurry transforms spontaneously to a solid wet body. The water-soluble copolymer acts both as a dispersing agent and as an auxiliary agent for spontaneous solidification. In this paper, the development history of spontaneous coagulation casting method is reviewed, the research progress is expounded, the influence factors are summarized, and the application prospect is prospected. The mechanism of the slurry consolidation is considered of two factors. The first one is the hydrophobicity change resulted from the ammonium ion migration. The hydrophobic parts of the polymer molecules assemble together binding the ceramic particles. The second factor is the high valence positive ions dissociated from ceramic particles because of surface hydrolysis or impurity dissolution. This novel method has been applied in manufacturing many kind of advanced ceramic, which is environmental friendly, easy operation, and low cost.

4:00 PM

(GFMAT-056-2019) Green synthesis of a synergetic structure of tellurium nanowires and metallic nanoparticles for biomedical applications

A. Vernet Crua*[1]; D. Medina Cruz[1]; T. J. Webster[1]; B. Zhang[1]

1. Northeastern University, Chemical Engineering, USA

Health care system is facing significant concerns nowadays such as antimicrobial resistance and cancer. New approaches should be considered, and nanotechnology has been found as a powerful solution to them. Current synthetic methodologies for production of nanoparticles, based on physicochemical procedures are known to be easy-to-get straightforward. Nevertheless, there are some drawbacks associated to them, such as the production of toxic by-products or the lack of biocompatibility of the products. Therefore, new methodologies are needed, and green chemistry offers itself as a suitable

*Denotes Presenter

and novel answer, achieving a safe and environmentally-friendly design, manufacture and use of chemical products. In this research, tellurium nanowires were synthesized using a green synthesis methodology (TeNWs). Then, they were used for the synthesis of metallic nanoparticles in an easy and straightforward method with no need of reducing agent that was completed within 1 minute of reaction. A novel structure composed by nanoparticles and nanowires - a synergy - was also obtained as a product of reaction. All compounds were c and charcaterized in terms of structure and composition. Besides, biocompatibility and anticancer tests of both structures – the synergy and the nanowires - with human tissue were accomplished, growing human dermal fibroblast (HDF) cells and melanoma cells in media in the presence of both nanosystems. After an incubation time of 5 days, the cell growth was analyzed using MTS assay. Furthermore, antibacterial properties were tested against Escherichia coli and Staphyloccocus aureus.

4:20 PM

(GFMAT-057-2019) Synthesis of TaC nano powders and its densification

W. Wang*[1]; Z. Fu[2]; H. Wang[1]; C. Liu[1]

1. Wuhan University of Technology, China
2. Wuhan University of Technology, State Key Lab of Advanced Technology for Materials Synthesis and Processing, China

Tantalum carbide (TaC) nano powders were synthesized by a novel method combining sol–gel method and spark plasma sintering (SPS) process using tantalum pentachloride ($TaCl_5$) and phenolic resin as the sources of tantalum and carbon, respectively. The gels of Ta-containing chelate with good uniformity and high stability were prepared by solution-based processing. The pyrolysis products with a structure of carbon coated Tantalum oxide (Ta_20_5) was obtained after pyrolyzed at 1073K. Further heat treatment by SPS allowed fast formation of TaC at a relatively low temperature (1673K). The TaC powders obtained at 1773K had an average particle size of about 40 nm and a low oxygen content of about 0.43 wt% at a comparably low C/Ta molar ratios of 4.25. The study on sintering densification behavior of TaC nano powder showed that synthesized TaC nano powder have a high sintering activity, dense TaC ceramics with 98.2%TD can be obtained by SPS sintered at 2173K and 80MPa.

G3: Crystalline Materials for Electrical, Optical and Medical Applications

Semiconductors

Room: Salon C
Session Chair: Yoshihiko Imanaka, Fujitsu Laboratories Ltd.

8:30 AM

(GFMAT-058-2019) Steps dynamics during high temperature solution growth of silicon carbide (Invited)

D. Chaussende*[1]; X. Xing[1]; Y. Yao[2]; T. Yoshikawa[2]

1. Univ. Grenoble Alpes, CNRS, SIMAP, France
2. The University of Tokyo, Institute of Industrial Science, Japan

4H-SiC (silicon carbide) is considered as the most relevant material for most of the power electronic applications, especially when very high power is required. As a general rule, performance gain is strongly linked to SiC crystal quality. The growth of SiC ingots from the top seeded solution growth (TSSG) method has emerged as an alternative to sublimation growth, for achieving ultra-high crystalline quality ingots. This requires a highly stable growth front, in the sense that the movement of atomic steps at the growing surface must be perfectly controlled. Recent achievements and open questions about the understanding of SiC step dynamics will be discussed. A special focus on step bunching, which is the main cause of interface destabilisation will be presented.

9:00 AM

(GFMAT-059-2019) Synthesis of SiC nanowires for high-efficiency electromagnetic wave absorption (Invited)

J. Kuang[1]; W. Cao*[1]

1. University of Science and Technology Beijing, China

SiC nanowire (SiC_w) is widely considered as a potential electromagnetic wave (EMW) absorbing material due to its good oxidation resistance and chemical inertness under high-temperature environment. However, the absorption ability is not satisfactory and should be effectively improved. In this work, Al, Fe, Mn and Ni doped SiC nanowires have been prepared. The experiment results indicated that both the dielectric and EMW absorption properties of the doped SiC nanowires were synergistically improved, which results in the enhanced conduction loss caused by doping and polarization loss induced by stacking faults consisting of 2H/3C heterostructures. In addition, the oxidation behavior and oxidation kinetics of the SiC nanowires were investigated at 600-1400 °C in air. Both the non-isothermal and isothermal oxidation kinetics were studied and the apparent oxidation energy was calculated to further describe the oxidation behavior of the SiC_W.

9:30 AM

(GFMAT-060-2019) Bone tissue engineering with piezoelectrical properties (Invited)

M. Nakamura*[1]

1. University of Turku, Institute of Biomedicine, Finland

The fundamental concept for bone tissue engineering is to use the natural biological responses in the host body. We explored the piezoelectrical properties of bone tissue in order to develop a rationale for improved ceramic bone grafts. Mechanical loading in bone tissue induces an electrical potential generated by piezoelectricity arising from displacement of collagen fibrils. The electrical potential is stored in collagen fibrils as well as apatite minerals. The stable electrical potentials stored in apatite minerals are enough to stimulate the osteogenic cells during bone remodeling. Furthermore, we observed that bone, when polarized electrically by external voltage, depolarized by two mechanisms. Specifically, carbonate incorporation and electrical charges in bone minerals are important factors in bone piezoelectricity. These factors modulated osteogenic cell behaviours such as the osteoclastogenesis of peripheral mononuclear blood cells and the differentiation of mesenchymal stem cells into osteoblasts. Understanding the mechanism of the effects of piezoelectrical properties on bone cells may allow us to design new biomaterials and select biomaterials for implantation that will last the lifetime of the recipient.

Optical Materials I

Room: Salon C
Session Chair: Didier Chaussende, CNRS/Univ. Grenoble Alpes

10:20 AM

(GFMAT-061-2019) Nonlinear materials for middle infrared OPCPA: State of the art and perspectives (Invited)

J. M. Delagnes*[1]

1. University of Bordeaux, CELIA, France

Middle infrared (MidIR) coherent sources with sub-300 fs durations and high average and/or peak power are highly attractive for strong field physics or secondary radiation production (XUV, THz), and find numerous applications such as ultrafast spectroscopy, or active imaging, Apart from direct laser emission, broadband MidIR radiation can be efficiently produced using nonlinear effects to convert ultrafast sources at near infrared central wavelength in order to reduced quantum defect and thermal heating. Current developments are lead not only on four wave mixing in photonic crystal fibres but also on second order effect (OPA, DFG) in nonlinear crystal We give a review of the characterization methods and MidIR OPCPA architectures based on well established (e.g. KTA) to emerging materials such as Langatate. We focus our discussion not only on the crystal properties such as homogeneity, nonlinear coefficients, and nonlinear refractive index and damage threshold, but also on the performances obtained in actual systems. We also discuss the present pumping sources and the trends in novel sources based on rare-earth (Ho, Tm) doped crystals or ceramics.

10:50 AM

(GFMAT-062-2019) Post-processing of CVD ZnSe transparent ceramics for infrared windows and nonlinear optics: The importance of stoichiometry and microstructure control (Invited)

R. M. Gaume*[1]; C. Goncalvez[1]; X. Chen[1]; K. A. Richardson[1]

1. University of Central Florida, CREOL, USA

Zinc selenide (ZnSe) has long been recognized as an important infrared (IR) material. This is due in parts to its broad transmission spectrum (0.2-14 μm), good thermal stability and the possibility of manufacturing large polycrystalline optics using chemical vapor deposition (CVD). In addition, its high second-order susceptibility values also make this material attractive for nonlinear interactions. The production of high-grade polycrystalline ZnSe windows, enabled by long-standing efforts and the relevance of this material for both strategic and industrial applications, is now being challenged by an ever-growing need for improved chemo-mechanical robustness. Similarly, the possibility of using transparent ZnSe ceramics in efficient, broadband nonlinear frequency converters, by way of random quasi-phase-matching (rQPM), requires better microstructure control than that which is currently available. This work investigates novel non-stoichiometric heat-treatments on CVD ZnSe ceramics aimed at producing hardened solid-solutions or composites, as well as controlled solid-state grain-coarsening for IR window and rQPM applications, respectively. Specifically, we show that the effect of heat-treatment atmospheres on hardening and the control of grain-size distribution can yield ceramics with improved mechanical and optical performance.

11:20 AM

(GFMAT-063-2019) Fabrication and characteristics of co-sputtered Ga-Sb-Te thin films

M. Bouska[1]; V. Nazabal[2]; T. Halenkovic[1]; J. Gutwirth[1]; P. Nemec*[1]

1. University of Pardubice, Czechia
2. Université de Rennes 1, France

During the last decades, the thin films from GeSbTe or AgInSbTe system have been deeply investigated. The main interest in these materials is their ability to transform quickly and reversibly from amorphous to crystalline phase and vice versa. Phase transition can be reversibly switched by varying the electric field or temperature when heating is performed using a laser pulse in optical recording applications. The unique characteristics of phase change Ge-Sb-Te materials are based on huge optical reflectivity (up to 30%) or electrical conductivity (several orders of magnitude) changes proceeding upon phase transition. In this work, we used radio-frequency co-sputtering as an advanced technique for thin films growth for the fabrication of inorganic materials being represented by Ga-Sb-Te thin films, as a possible alternative to Ge-Sb-Te system. The characterization of deposited thin films in as-deposited state (amorphous phase) as well as in crystalline state (induced by thermal annealing) was performed exploiting atomic force microscopy, scanning electron microscopy with energy-dispersive X-ray analysis, X-ray diffraction, electrical resistivity, and variable angle spectroscopic ellipsometry data. The results are discussed in relation with the chemical composition of the fabricated Ga-Sb-Te thin films. The financial support of the Czech Science Foundation under the project No. 18-03823S is greatly acknowledged.

11:40 AM

(GFMAT-064-2019) Gd doped YAG transparent ceramics with an ultraviolet emission

G. Zhang*[1]; Y. Wu[1]

1. Alfred University, Materials Science, USA

Gd^{3+} doped YAG transparent ceramic is a good candidate in UV emitting applications and was synthesized by spark plasma sintering through a solid state reaction using TESO as a sintering additive. X-ray diffraction, scanning electron microscope, photoluminescence (PL), and UV–Vis–NIR were used to characterize the synthesized ceramic materials. The Gd^{3+} doped YAG ceramic material after post annealing exhibits UV emission at 312nm under an excitation at 273nm. The in-line transmission for 1% at Gd doped YAG transparent ceramic was 70.19% and 78.55% at 550 nm and 800 nm, respectively. The research work shows that Gd^{3+} doped YAG transparent ceramics with ultraviolet emissions is considered as a promising material for applications of solid-state UV devices.

Optical Materials II

Room: Salon C

Session Chairs: Jean-Christophe Delagnes, University of Bordeaux; Inka Manek-Hönninger, University of Bordeaux

1:30 PM

(GFMAT-065-2019) Fluoride Ceramic Phosphors for LED Lighting (Invited)

N. Cherepy*[1]; R. Osborne[1]; Z. M. Seeley[2]; S. A. Payne[1]; W. Beers[3]; W. Cohen[3]; D. Schlagel[4]; H. Comanzo[5]; A. Srivastava[5]

1. Lawrence Livermore Nat'l Lab, Chemistry and Materials Science, USA
2. Lawrence Livermore Nat. Lab, Chemical Sciences Division, USA
3. Current by GE, USA
4. Ames Laboratory, USA
5. GE Global Research, USA

New phosphor ceramics that convert blue Light Emitting Diode (LED) light into a tunable white light spectrum can be produced by consolidating multiple phosphors into a fully dense translucent ceramic. Use of a fluoride matrix facilitates formulation of multi-phosphor ceramics for white light emission offering both high CRI and efficacy, and can be designed to produce various correlated color temperatures. Phosphor ceramics offer improved environmental stability and thermal conductivity for use with high blue light pump flux, since heat generated may be efficiently conducted away, minimizing thermal quenching at high power. In addition, the translucency of the ceramic provides for a longer excitation pathlength in the phosphor, allowing doping level to be reduced, mitigating concentration quenching and improving thermal stability of luminescence, known to be exacerbated at high dopant concentrations. Our team of scientists at LLNL, GE and Ames Laboratory is developing new LED lighting structures based on this new class of phosphor ceramics.

2:00 PM

(GFMAT-066-2019) Comparison between sintered crystal and stoichiometric glass for phosphor application (Invited)

H. Masai*[1]

1. National Institute of Advanced Industrial Science and Technology (AIST), Department of Materials and Chemistry, Japan

For the material design of such activators, tailoring the coordination in a crystal is easier than that in amorphous (glass) materials exhibiting a random network. In addition, because the random network might possess local defects that induce non-radiative relaxation, glasses are not considered attractive as host materials of inorganic phosphors. However, if the luminescence efficiency in glass is comparable to that in the crystal, a good formability of the glass will be considerably advantageous for industrial applications, because it allows the fabrication of complex shapes in various material sizes. From this viewpoint,

a glass with a chemical stoichiometric composition equivalent to that of a phosphor crystal will be a good candidate with good formability and relatively low fabrication cost. In the present study, the emission properties of several glasses with the stoichiometric chemical composition of crystals are presented. The differences due to the network randomness will be discussed on the day.

2:30 PM

(GFMAT-067-2019) Electro-optical device with tunable coloration and transparency using colloidal core/shell nanoparticles (Invited)

J. Han*[1]; E. Lee[1]; M. Freyman[1]; E. Feigenbaum[1]; A. Pascall[1]; J. Kuntz[1]; M. Worsley[1]; T. Y. Han[1]

1. Lawrence Livermore National Lab, USA

Amorphous photonic structures exhibit interesting optical properties such as non-iridescent angle-independent structural colors and produce striking structural coloration are easily found in various living organisms such as birds, insects, sea animals, and even in plants. Here, we demonstrate colloidal assemblies of engineered amorphous photonic materials, using pigmentary core/shell nanoparticles, exhibiting non- iridescent and tunable colors. Using these photonic materials, structural colorations and their dynamic tunability are demonstrated. Furthermore, we successfully fabricated novel transparency tunable device in response to electric stimuli using colloidal spherical core/shell nanoparticles. The observed transparency change is attributed to structural ordering of nanoparticle assemblies and thereby modify the photonic band structures. The resulting colors and transparency can be manipulated by shell thickness, particle concentration, device fabrication and external electrical stimuli, which will be discussed in the presentation, This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

3:20 PM

(GFMAT-068-2019) Zirconia phosphor for biological temperature sensing probe: Afterglow property and its doping effect

S. Goto*[1]; M. Ohashi[1]; N. Terakado[2]; Y. Takahashi[2]; Y. Nakajima[3]; N. Onoue[4]; T. Shinozaki[4]; T. Fujiwara[2]

1. Tohoku University, Japan
2. Tohoku University, Department of Applied Physics, Japan
3. Daiichi Kigenso Kagaku Kogyo Co., Ltd., Japan
4. Sendai Med. Center, Japan

In medical field, novel innovation for non-invasive and site-selective temperature detection in the deep parts of human-body has been required. Our research group has attempted to develop the temperature-detecting method and its probe based on photophysical phenomena, e.g., afterglow and photo-stimulated luminescence, so far. Particularly, "biological window", which corresponds to the wavelength region in ~650–1000 nm, has been focused on because the light can transmit in the living body: We have focused on a less-toxic and stable compound, i.e., zirconia; ZrO_2 as a temperature-sensing probe. Although ZrO_2 shows an excellent afterglow property without any dopants, its afterglow wavelength is non-compatible with the biological window. Therefore, we have examined the doping-effect on afterglow property in the ZrO_2, and have succeeded in shifting the afterglow wavelength in red-region.

3:40 PM

(GFMAT-069-2019) Synthesis and characterization of PbS Quantum Dots/perovskite solar cells

A. Nemati*[1]; A. Attari Navab[1]

1. Sharif University of Technology, Materials Science & Engineering, Islamic Republic of Iran

Quantum dots (QD) have emerged as new generation of nanomaterials with special photoelectric, Photovoltaic, photocatalytic and photoluminescence characteristics. In this research, the effects of incorporating PbS Quantum Dots (PSQD) in hybrid MAPbI3 perovskite solar cells were studied. The PbS QDs are deposited using the successive ionic layer adsorption and reaction (SILAR) method. Then, the effects of the SILAR coating cycle on light absorption were studied. During the synthesis of PbS QDs, the effect of number of cycles and concentration of anionic and cationic solutions on the properties and structure of PbS QDs were evaluated. The effects of growth factor of synthesized PbS QDs on microstructural features of perovskite (MAPbI3) and improvement of the performance of adsorbent materials in perovskite solar cells were evaluated. The results showed that the increase in immersion time led to the completion of the $MAPbI_3$ processor synthesis with mean grain size of the $MAPbI_3$ crystals of 0.66 μm. The mean PbS grain size at a concentration of 0.20M solution in 1, 2, 4 cycles were 6.38, 7.20, 7.83nm; respectively and the absorption edge of samples was extended to 900nm. The nature of agglomeration in PbS QDs changes the growth direction.

4:00 PM

(GFMAT-070-2019) Rare Earth Doped Crystals for Microwave-Optical Quantum Interfaces (Invited)

P. Goldner*[1]

1. Chimie ParisTech, France

Quantum technologies are developed to overcome classical limits in communication and processing but also in new areas like sensing, imaging, and simulations. They will impact all aspects of life by allowing e.g. ultra-secure communications, simulation of complex molecules, or new medical bio-imaging techniques. Many quantum systems are investigated for specific tasks. The next major challenge is to overcome the limits of single systems by associating different quantum systems in hybrid architectures, each selected for its specific properties. Optical interconnection of these systems will also be necessary to further develop functionalities in a global 'quantum internet'. Crystals doped with paramagnetic rare earth ions could play a pivotal role in this scheme by offering a solid-state platform that enables efficient coupling between microwave and optical photons. This has a strong interest in connecting superconducting quantum processors with optical networks to create e.g. distributed quantum processing. In this paper, we will discuss recent advances in this field, including the development of a new system $Yb^{3+}:Y_2SiO_5$ that shows exceptional optical and spin coherent properties.

4:30 PM

(GFMAT-071-2019) Femtosecond direct laser writing in Calciumfluoride crystals (Invited)

I. Manek-Hönninger*[1]; W. Gebremichael[1]; Y. Petit[2]; L. Canioni[1]

1. University of Bordeaux, CELIA, France
2. University of Bordeaux, ICMCB/CELIA, France

Femtosecond direct laser writing (DLW) allows for realizing a vast range of photonic devices which is a driving force behind industrial interest for rapid prototyping of optical components. Crystals are of special interest due to their crystallographic properties, and some of them can serve as active media when doped with rare earth ions. An interesting candidate is CaF_2, which is cubic and an already widely used as host for high power laser media. As a step towards very compact waveguide lasers based on CaF_2, we realized waveguides written in undoped crystals. The waveguides are single mode and based on double-tracks with negative index change. Moreover, we study the influence of the polarization and the writing direction with respect to the induced modifications by femtosecond DLW inside these crystals along the damaged tracks, and we observed type II and smooth modifications depending on the DLW configurations.

5:00 PM

(GFMAT-072-2019) Upconverting nanoparticles for seeing and delivering drugs inside the body (Invited)

G. Jalani[1]; V. Tam*[1]; D. Rosenzweig[1]; R. Naccache[3]; L. Haglund[1]; F. Vetrone[2]; M. Cerruti[1]

1. McGill University, Canada
2. Institut National de la Recherche Scientifique, Université du Québec, Centre Énergie, Matériaux et Télécommunications, Canada
3. Concordia University, Chemistry and Biochemistry, Canada

When upconverting nanoparticles (UCNPs) are hit with near infrared (NIR) radiation, they can upconvert it to higher frequencies spanning the NIR, visible and UV. This is particularly useful in bioapplications: since NIR light can penetrate a few centimeters through the skin, UCNPs can be used in-vivo as probes or nano-antennas. The rare-earth oxide core of UCNPs is usually coated with a silica layer to make it hydrophilic. This allows the NPs to be dispersed inside biologically-friendly materials, and use them as probes to track, for example, hydrogel degradation. Adding to this layer a thin organic coating including photocleavable links extends the function of UCNPs to a theranostic platform able to deliver molecules on-demand, with precise and immediate control over their release. This talk will explore both functions of UCNPs (probes and delivery vehicles) and discuss prospects of these particles for clinical applications.

G5: Advanced Functional Materials, Devices, and Systems for Environmental Conservation, Pollution Control and Critical Materials

Advanced Functional Materials, Devices, and Systems III

Room: Trinity III

Session Chairs: Tetsuo Uchikoshi, National Institute for Materials Science; Yoshiteru Itagaki, Ehime University

8:55 AM

(GFMAT-073-2019) Preparation of a-$LiAlO_2$ with layered-NaCl type structure by sol-gel method and the electrochemical property

Y. Arachi*[1]; A. Shibata[1]

1. Kansai University, Chemistry and Materials Engineering, Japan

Developments of positive electrodes with high capacity for Li-ion batteries have been extensively investigated. We have focused on the possibility for oxide ions of metal oxides to participate in the electrochemical reaction, which is different from that of popular positive electrodes such as $LiCoO_2$ or $LiFePO_4$. Although the first principle calculation of a-$LiAlO_2$ suggested the reaction, the experimental results have been limited because the heating during conventional solid state reaction makes the structure disorder easily. Therefore, we have adopted a-$LiAlO_2$ to investigate the electrochemical activity experimentally and examined the preparation by sol-gel method. A single a-$LiAlO_2$ phase with layered-NaCl type structure was obtained by polyvinylpyrrolidone(PVP)-assisted sol-gel method. We have confirmed that the crystal structure was identical to that of $LiCoO_2$ by Rietveld analysis. The electrochemical testing indicated that the electrochemical activity was induced by co-existing $LiCoO_2$. In this presentation we will present a role of PVP in preparation of a-$LiAlO_2$ and the electrical conductivity, mainly ionic conductivity, and then discuss the electrochemical activity.

9:10 AM

(GFMAT-074-2019) Synthesis and Property of Garnet-Type Fast Lithium Ion Conducting Materials (Invited)

J. Akimoto*[1]; K. Kataoka[1]

1. AIST, Japan

All solid state Li-ion batteries using solid oxide electrolyte have attracted attention as next-generation batteries without inflammable organic liquid electrolytes. Among many candidates of Li-ion conducting oxide materials as solid electrolyte for all solid state LIB, the garnet-type $Li_7La_3Zr_2O_{12}$ and its chemical derivatives have been investigated so as to improve electrochemical performance. We recently focused on the Ta-substituted $Li_7La_3Zr_2O_{12}$ materials having a relatively higher Li-ion conductivity at room temperature. We synthesized sintered body and single crystal samples of $Li_{6.5}La_3Zr_{1.5}Ta_{0.5}O_{12}$, and determined precise structural and electrochemical properties. A relationship between the detailed Li-ion arrangement in the loop structure constructing by the garnet framework and the Li-ion conductivity will be presented.

9:35 AM

(GFMAT-075-2019) Novel Calcium Ion Conducting Solids with NASICON-type Structure (Invited)

N. Imanaka*[1]

1. Osaka University, Applied Chesistry, Japan

Divalent calcium ion conducting solids with the three dimensional NASICON-type structure, $(Ca_xHf_{1-x})_{4/(4-2x)}Nb(PO_4)_3$ [1], was successfully prepared by introducing divalent calcium cations into the $HfNb(PO_4)_3$ mother lattice. The existence of three kinds of high valence cation of Hf^{4+}, Nb^{5+}, and P^{5+} realized the effective reduction of electrostatic interaction between Ca^{2+} and O^{2-}, in the structure. The NASICON-type $(Ca_{0.05}Hf_{0.95})_{4/3.9}Nb(PO_4)_3$ solid possesses considerably high Ca^{2+} cation conductivity and low activation energy in comparison with those of previously reported NASICON-type $Ca_{0.5}Zr_2(PO_4)_3$ [2] solid electrolyte. The conductivity of $(Ca_{0.05}Hf_{0.95})_{4/3.9}Nb(PO_4)_3$ was considerably higher than that of the $Ca_{0.5}Zr_2(PO_4)_3$ [2] solid in all the temperature range examined. In addition, the activation energy (E_a = 55.8 kJ mol^{-1}) for Ca^{2+} ion migration is considerably lower than that (E_a = 146 kJ mol^{-1}) of $Ca_{0.5}Zr_2(PO_4)_3$ [2]. Since the Ca^{2+} ion concentration in the NASICON-type solids is similar, the higher Ca^{2+} ion conductivity and the lower activation energy for the present $(Ca_{0.05}Hf_{0.95})_{4/3.9}Nb(PO_4)_3$ solid are caused by the effective reduction of electrostatic interaction between Ca^{2+} and O^{2-} ions, by the co-existence of higher valence cation of Hf^{4+}, P^{5+} and Nb^{5+} compared with Ca^{2+}.

Advanced Functional Materials, Devices, and Systems IV

Room: Trinity III

Session Chairs: Nobuhito Imanaka, Osaka University; Junji Akimoto, AIST

10:20 AM

(GFMAT-076-2019) Advanced Hydride Research for Energy Device Application (Invited)

S. Orimo*[1]

1. Tohoku University, Japan

Complex hydrides exhibit various energy-related functions as shown below; such as high-density hydrogen storage and microwave absorption for future fuel cell technologies, as well as fast-ionic conduction for energy devices. In the presentation, recent studies on lithium/sodium superionic conduction and development of all-solid-state lithium-ion battery devices (both the high-energy-density and high-thermal-durability types) using complex hydrides are to be explained.

10:50 AM

(GFMAT-077-2019) Oxygen Separation from Air using BSCF-based Mixed Conductor Membrane (Invited)

T. Uchikoshi*[1]; K. Ishii[3]; A. Stevenson[2]; C. Tardivat[2]

1. National Institute for Materials Science, Japan
2. Saint-Gobain, France
3. Hokkaido University, Japan

Mixed Ionic-Electronic Conducting (MIEC) membrane is focused on gastight oxygen permeable membrane (OPM). MIEC allows oxygen diffusion through vacancies in the crystal lattice, which is charge-compensated by intrinsic electronic conductivity. Therefore, such membranes show infinite selectivity, in principle, resulting a production of 100% pure oxygen. It does not need any external electrical supply due to the inner short circuit by electronic conduction. Perovskite-type Ba-Sr-Co-Fe-O (BSCF) exhibits high mixed conductivity. Therefore OPM using BSCF material exhibits high oxygen permeability. However the oxygen permeation flux is not enough high for practical use. Therefore, a remarkable improvement in the oxygen permeation rate is strongly demanded. It is important to design asymmetric structure composed of porous high reaction area and dense, thin membrane, in order to improve the oxygen permeability. In this study, a thin, dense BSCF layer was fabricated on a porous BSCF support by the electrophoretic deposition (EPD) method. Wheat starch powder was used for a pore forming agent of the porous support. The dense/porous asymmetric membrane was obtained after the deposition of a thin layer of on the porous support, followed by sintering at 1100 °C for 3h. The interface between the two BSCFs was well-bonded and crack-free. Oxygen permeation properties will be reported in the presentation.

11:15 AM

(GFMAT-078-2019) Ammonia fueled solid oxide fuel cells with Ni based anodes (Invited)

Y. Itagaki*[1]; J. Cui[1]; Y. Tani[1]; H. Yahiro[1]

1. Ehime University, Department of Sicence and Engineering, Japan

Ammonia is a promised hydrogen carrier, because it contains high density of hydrogen, consisits of only hydrogen and nitrogen and is easily liqudified. For this reason, solid oxide fuel cells (SOFC) fueled with ammonia has been extensively studied so far. In this study we developed ammonia fueled SOFCs with oxide ionic electrolytes. In the case of the oxide ion conducting cells, Ni-Sm2O3-CeO2 anode with 10 wt% Ni content exhibted high performance in 30%NH3 fuel. High Ni content enlarged electric conductivity but simultaneously induced Ni aggregation which decreased a catalytic actiuvity. Adding BaCe0.8Y0.2O3 protonic conducting electrolyte into the anode significantly surpressed the Ni aggregation even higher Ni contents.

11:40 AM

(GFMAT-079-2019) An Internet of Things based multi-purpose ceramic sensor for ultra-high temperature and heat flux sensing

A. Purwar[1]; V. Sharma*[2]

1. Indian School of Business, India
2. Indian Institute of Science, Material Research Centre, India

The next-generation industrial machinery, viz., gas turbines, engines and boilers will rely heavily on smart data acquisition and monitoring to meet performance and control requirements. These machines also require precise measurement and forecasting of temperature and heat flux for structural health monitoring and smart control. This necessitates the development of a robust sensor system which can measure these parameters and transmit them in real time. In our proposed system, there are 3 hardware components viz. sensor probe, electronics for wireless transmission and enclosure for housing electronics. First, an affordable Internet of Things (IoT) based sensor probe and a sensor housing developed out of Zirconium diboride and YSZ multi-layer ceramic composite has been designed. The sensor acquires and transmits data in real time to cloud (web server). The temperature-cum-heat flux sensor probe and electronics instrumentation enclosure have been designed using rigorous finite element modelling. The sensor and enclosure can withstand temperature and pressure up to 2500K and 100 bars respectively. Besides, data acquisition and forecasting software have been developed for visualization and forward estimation of temperature and heat flux. The software has been made open source (https://github.com/Ammadus/Data-acquisition-and-forecasting-tool). Thus, the proposed sensor based on multi-layer ceramic system provides real-time measurement in the range 300-2500K without any cooling.

Advanced Functional Materials, Devices, and Systems V

Room: Trinity III
Session Chairs: Yoshinobu Nakamura, Department of Advances Materials Science, Faculty of Frontier Science, The University of Tokyo; Kiyofumi Katagiri, Hiroshima University

1:30 PM

(GFMAT-080-2019) Theoretical prediction of 4f-5d transition energy of Ce^{3+} in garnet-type oxides based on the combination of first-principles calculation and machine learning (Invited)

K. Ogasawara*[1]

1. Kwansei Gakuin University, Department of Chemistry, Japan

Since the Ce^{3+}-doped crystals are utilized as various optical materials such as phosphors for white LEDs, it is important to predict the electronic structures of Ce^{3+} in given host crystals for theoretical design of novel optical materials. The first-principles molecular orbital (MO) calculations are quite useful to predict the electronic structures. However, complicated calculations using large clusters are usually required for accurate predictions. In this work, in order to establish a more efficient method to predict the 4f-5d transition energy, we combined the first-principles MO calculations using relatively small model clusters with the machine learning technique. The first-principles calculations of the electronic structures of Ce^{3+} in various garnet-type oxides have been performed based on the relativistic DV-Xα MO calculations using the model clusters consisting of the central Ce^{3+} ion and the first-neighbor O^{2-} ions. The regression formula of the 4f-5d transition energy of Ce^{3+} based on the predictor variables related to the electronic states and the local structures has been derived by the machine learning using WEKA. The results indicated that the theoretical prediction based on the small clusters was significantly improved by consideration of the net charge of Ce^{3+} as a predictor variable.

1:55 PM

(GFMAT-081-2019) Deep red phosphors based on fluorine doped lithium aluminate with the luminescent centers of 3d transition metals (Invited)

Y. Matsushima*[1]; R. Kobayashi[1]; C. Sato[1]; Y. Kamada[1]; K. Sato[1]; H. Tamura[1]; H. Kominami[4]; K. Hara[3]; M. Kakihana[2]

1. Yamagata University, Chemistry and chemical engineering, Japan
2. Tohoku University, Institute of Multidisciplinary Research for Advanced Materials, Japan
3. Shizuoka University, Research Institute of Electronics, Japan
4. Shizuoka University, Electronics and Materials Science, Japan

Deep red phosphors based on fluorine doped lithium aluminate was proposed with the luminescent centers of Mn^{4+}, Fe^{3+}, and Cr^{3+}. The compositional analysis indicated $Al_{4.85}Li_{1.15}F_{0.10}O_{7.80}$ (ALFO) for this host compound, although a slight deviation was recognized in the chemical composition. ALFO is a related compound to spinel type $LiAl_5O_8$. The cation arrangement of Li^+ and Al^{3+} in $LiAL_5O_8$ is regularly ordered in the tetrahedral and octahedral sites in the spinel-type lattice, while Li^+ and Al^{3+} were randomly distributed over the cation sites in ALFO and the fluorine substitution for the oxygen atoms promoted the structural disordering. Each of Mn^{4+}, Fe^{3+}, and Cr^{3+} in ALFO brought the deep red emission with the CIE coordinates of

(0.704, 0.280) for Mn^{4+}, (0.703, 0.279) for Fe^{3+}, and (0.729, 0.271) for Cr^{3+}. Among these luminescent centers, the emission peak of Mn^{4+} arose on the shortest wavelength side with the peak top at 661 nm. Fe^{3+} and Cr^{3+} respectively showed the rather broad peak centering around 690 nm and the characteristic twin peak with the tops at 705 and 715 nm.

2:20 PM

(GFMAT-082-2019) Development of 3R Process for Electrical and Optical Ceramics Components by Using Photo-Reaction Process (Invited)

T. Tsuchiya*[1]; T. Manabe[1]; N. Kijima[1]; Y. Uzawa[1]

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

In most case, as a ceramic materials or components is manufactured by a high temperature processing, a large amount of CO_2 is generated. To construct eco-society for next generation, it is necessary to develop a new manufacturing processing for ceramic material and components without a large amount of CO_2 generation. In addition, in order to protect the environment and critical resources, an innovative circulation cycle of the ceramics materials and components in devices is also needed. Commonly, these components for green devices are manufactured using mixture resin or glass of the functional ceramics' materials. Such a composite material, for example, leads to makes recycling difficult. For this aim, we developed low temperature process for oxide thin film and proposed the new 3R process for electrical and optical components. In this process, a electronic components (resistor) can be fabricated on a plastic substrate without using glass or resin with not only excellent properties but also durability and recyclability. In this presentation, we will introduce photo reaction process for the ceramics thin film growth such as RuO_2 thin films (a high heat resistant electronic component for SiC power electronics) or ITO or SnO_2 thin films (transparent conductive film) or VO_2 thin film for smart window.

2:45 PM

(GFMAT-083-2019) Investigation on titania modified with first-low transition-metal oxides nanoparticles for water photooxidation under visible light

M. Okazaki*[1]; K. Maeda[1]

1. Tokyo Institute of Technology, Japan

TiO_2 is one of the best-known heterogeneous photocatalysts for water splitting. However, it cannot absorb visible light because of its large band gap. To address this problem, we developed a new water oxidation system: titania modified with cobalt oxide (CoO_x) nanoparticle. This material can absorb entire-region of visible light. It has been shown by photoelectrochemical measurements that electron transition from CoO_x to conduction band of TiO_2 occurred. Therefore, the electron interaction between the loaded Co species and the TiO_2 support is supposed to be important in this system. Here we investigated the first-low transition-metal oxides (MO_x, M = Mn, Fe, Ni) as alternatives to CoO_x to expect that similar effects working as water oxidation photocatalysts under visible light. As a result, we revealed that all MO_x/TiO_2 except NiO_x/TiO_2 did not show photocatalytic activity although all of them possessed visible light absorption capability. We also investigated the catalytic abilities for water oxidation of MO_x to clarify the photocatalytic inactiveness despite of those light absorption capability. It was confirmed that CoO_x had the highest ability to oxidize water among the tested MO_x. This result suggests that not only wide range absorption capability but intrinsic catalytic performance of MO_x is important to this MO_x/TiO_2 photocatalysis system.

Advanced Functional Materials, Devices, and Systems VI

Room: Trinity III

Session Chairs: Tetsuo Tsuchiya, National Institute of Advanced Industrial Science and Technology (AIST); Kazuyoshi Ogasawara, Kwansei Gakuin University

3:20 PM

(GFMAT-084-2019) Optical Observation of the Current Carrying Degradation Process of a RuO_2 resistor under a Severe Usage Environment (Invited)

Y. Nakamura*[1]; M. Miyayama[1]

1. Graduate School of Engineering, The University of Tokyo, Applied Chemistry, Japan

Ruthenium oxide (RuO_2) thick-film resistor is a leading candidate for the resistor element for next-generation high-power module. However, resistor elements used for a high-power module involve the risk of the acceleration aging of their electrode parts due to the operation at high temperature. Here, we devised a simple and noninvasive method for detecting the local degradation of a RuO_2 resistor by the analysis of UV-VIS-IR microspectroscopic data and got the information about the degradation mechanisms triggered by the long-term use in a harsh environment. The results of local carrier density mapping obtained from the reflectance data revealed that an unexpected change in resistance during standing in a high temperature (>523K) environment was partially due to the annihilation of the originally existing higher carrier density areas in the vicinity of the Ag electrode- RuO_2 thick-film interface. Under the current-loading condition, the degradation mechanisms were rather complex and it is further revealed that long range diffusion of Ag accompanied by the anodic corrosion of the electrode caused an unexpected decrease in resistance. Based on the above experimental results, we are going to establish the method for preventing both thermal and current carrying degradation of a RuO_2 resistor for the use of severe usage conditions.

3:45 PM

(GFMAT-085-2019) Change in mechanical properties of dielectric ceramics on annealing contacted with the other isomorphic ceramics (Invited)

A. Kishimoto*[1]; K. Nomura[1]; T. Teranishi[1]; H. Hayashi[1]

1. Okayama University, Graduate School of Natural Science and Technology, Japan

The formation of surface compression layers was confirmed on two sets of dielectric ceramics, barium titanate –barium zirconate and titanium oxide –tin oxide, through the change in mechanical properties of titanium based oxide accompanied by an interdiffusion. On the interdiffusion of barium titanate -barium zirconate, it was confirmed that the flexural strength of the diffused sample was about 10% higher than that of the annealed sample. The hardness of the untreated, annealed sample remained constant irrespective of test force, although the diffused sample showed an increase in hardness by decreasing the test force. Improvement in flexural strength and hardness suggests the formation of a surface compression layer of barium titanate by the interdiffusion with barium zirconate. In the case of titanium oxide- tin oxide, on the other hand, no significant strength improvement cannot be seen in usual annealing, however, the flexural strength has improved through a millimeter-wave irradiation heating.

4:10 PM

(GFMAT-086-2019) Enhancement of piezoelectric response in {100}-oriented films using extrinsic contribution (Invited)

H. Funakubo*[1]; N. Oshima[1]; H. Inoue[1]; Y. Ehara[1]; T. Shimizu[1]; H. Uchida[2]

1. Tokyo Institute of Technology, Japan
2. Sophia University, Japan

Piezoelectric films have been widely investigated for various applications such as inkjet printer and gyro sensor and so on. However, their piezoelectric response is generally lower than that of the sintered body due to the clamping from the substrates. To overcome this disadvantage, we propose the reversible domain switching or phase transition under applying an electric field. In this case, we can use the clamping from the substrates as a positive effect. In my presentation, I introduce our novel concept to enhance the piezoelectric properties and show the obtained results.

G8: Advanced Batteries and Supercapacitors for Energy Storage Applications

Theory

Room: Salon D
Session Chair: Naoaki Yabuuchi, Tokyo Denki University

8:30 AM

(GFMAT-088-2019) Design principles for layered and spinel intercalation compounds for Li, Na and K-ion batteries (Invited)

A. Van der Ven*[1]

1. University of California Santa Barbara, Materials, USA

Layered and spinel crystal structures have proven very successful as host materials for Li, Na and K intercalation processes, as occurs in the electrodes of rechargeable batteries. Variations in anion chemistry (sulfur versus oxygen) and transition metal chemistry of the host can have a dramatic impact on the electrochemical properties of intercalation compounds. In this talk I will review insights about the link between chemistry and electrochemical properties of layered and spinel hosts as derived from first-principles studies. First-principles statistical mechanics approaches are capable of predicting a range of important electrochemical properties, including voltage profiles, ionic diffusion coefficients and mechanical properties. This makes it possible to systematically vary crystal structure and chemistry to elucidate how such variations affect properties.

9:00 AM

(GFMAT-089-2019) Methodological issues in DFT based modeling of active electrode materials for advanced metal-ion batteries (Invited)

S. Manzhos*[1]

1. Institut National de la Recherche Scientifique, Centre Énergie Matériaux Télécommunications, Canada

Ab initio modeling is widely used to rationalize the performance of active electrode materials in metal ion batteries as well as to rationally select or design promising materials for storage of Li, Na, K, Mg, Al and other types of cations. It faces certain methodological challenges such as reproducing correct bandstructure, phase ordering, or treatment of van der Waals interactions in layered oxides. An important issue is the conceptual framework in which redox processes are understood. I will share how in my group we dealt with the above issues when modeling different phases of titania and vanadia (layered and non-layered) intercalated with Li, Na, Mg (as well as K and Al in the case of vanadia) i.e. atoms of different valence and cation size. I will highlight use of effective localized basis sets and differences in bandstructure behavior with respect to the amount of Hubbard correction with different basis types, effect of intercalation on phase ordering, and recommended ways to apply a posteriori vdW corrections. I will highlight cases where the electron donated by the intercalant alkali atom is distributed over two transition metal atoms bridged by oxygen rather than localized on a single d state. Finally, I will demonstrate inadequacy of formal oxidation states as the basis for understanding the mechanism in intercalated oxides.

9:30 AM

(GFMAT-090-2019) Thermodynamics and Ion Transport of Multivalent Cathode Materials (Invited)

P. Canepa*[1]

1. National University of Singapore, Materials Science and Engineering, Singapore

Multi-valent (MV) batteries that replace Li+ ions with MV cations, including Mg2+, Zn2+ and Ca2+ represent a promising approach to meet the high energy density requirements of the next generation of electrical devices. Perhaps the most pressing challenge in achieving high energy density MV-ion systems is to develop suitable cathode materials and conductors with a significant voltage and high MV-ion transport. To date, there have been limited examples demonstrating the feasibility of rechargeable MV batteries, and among them, most of the focus has been on Mg technology. The feasibility of a battery technology based on MV intercalation is not yet clear. The cathode represents a critical component of this technology. I will present a detailed analysis, based on first-principles DFT calculations, of MV intercalation in promising candidates, including the MVB2X4 system (with B = TM and X=O or S) and the polymorphs of layered V2O5. I will show that computational materials science is a powerful tool to pave the development and optimization of materials for energy dense MV batteries.

All-Solid-State-Batteries

Room: Salon D
Session Chair: Mickael Dollé, Université de Montreal

10:20 AM

(GFMAT-091-2019) Development of Flexible Composite Solid Electrolyte and Quasi-solid Composite Cathode for Practical Realization of Solid-state Lithium-ion Batteries

K. Kanamura*[1]; M. Shoji[1]; E. Cheng[1]

1. Tokyo Metropolitan University, Graduate School of Urban Environmental Sciences, Japan

Lithium-ion conducting solid electrolytes are key materials for realizing all-solid-state lithium-ion batteries. In particular, oxide solid electrolytes such as LLZO are attractive due to their excellent thermal, electrochemical and chemical stability. However, they are easy to break upon stress and hard to form an intimate interface with cathode layer. Thus, a flexible solid electrolyte is required, because its flexible nature is effective against stress. Also, techniques for forming the interface are necessary. For these requirements, we have developed a flexible composite electrolyte sheet and a quasi-solid composite cathode. Both are filled with ionic or solvate ionic liquid. Recently, we investigated about a LLZO-based composite sheet and a $LiCoO_2$-based composite cathode. Thickness and ionic conductivity of the LLZO sheet were ~100 μm and 0.6 mS cm^{-1}, respectively. Since the $LiCoO_2$ composite cathode was prepared from a slurry, sheet preparation was very easy. An electrochemical cell with the $LiCoO_2$ composite cathode and LLZO pellet showed good cycling performance for 100 cycles. Moreover, we have fabricated a solid-state cell consisting of the LLZO sheet, the $LiCoO_2$ composite cathode sheet and a lithium foil. The full cell operated and delivered a discharge capacity of 100 mAh g^{-1} at 60 °C.

10:55 AM

(GFMAT-092-2019) All-Solid-State Sodium Battery using electrode materials with different sintering temperature (Invited)

T. Kobayashi*[1]

1. Central Research Institute of Electric Power Industry, Japan

All-solid-state batteries have any attractive characteristics of high safety, good reliability, and long life-durability. However, weak contact between hard oxide-based materials formed by cold pressing prevents lithium-ions or sodium-ions from conducting at the electrode/electrolyte interface. Thus, an appropriate sintering process is necessary to form the strong contact and to ensure the effective conduction of lithium-ions or sodium-ions at the interface. However, a few combinations of the positive and the negative electrode materials can work electrochemically in the sintered batteries using the identical electrode active material (ex. $Na_3V_2(PO_4)_3$) or electrode materials with approximate sintering temperatures for both electrodes. It has been a weakness to restrict electrode choice in oxide-based all-solid-state batteries. In this study, a new process is proposed to fabricate an all-solid-state battery using different electrode active materials as positive and negative electrodes with different sintering temperatures. The battery is fabricated by jointing two pellets including the positive and negative electrode materials, respectively, and using an inorganic adhesive material. The detailed process and the battery performance will be discussed.

11:25 AM

(GFMAT-093-2019) Oxide-based All-Solid-State Rechargeable Batteries using Room Temperature Ceracmis Densification Technology (Invited)

Y. Iriyama*[1]

1. Nagoya University, Japan

Electrode-solid electrolyte interface is a key issue to develop adcvanced all-solid-state batteries (SSBs). Here, we will show that dense electrode-solid electrolyte composite is prepared by aerosol deposition (AD), a room temperature ceramics densification technology, and that the composite electrode works well in oxide-based SSBs combined with LLZ and Li metal anode. In addition, a unique-type Li-free thin film batteries specifically prepared by the AD technology will be also introduced.

Anodes: Li-ion and Na-ion Battery

Room: Salon D

Session Chair: Valerie Pralong, CNRS ENSICAEN

1:30 PM

(GFMAT-094-2019) Pristine or Highly Defective? Understanding the Role of Graphene Structure for Stable Lithium Metal Plating (Invited)

D. Mitlin*[1]

1. University of Alberta and NINT NRC, Chemical and Materials Engineering, Canada

We are the first to examine the role of graphene host structure/chemistry in plating-stripping in lithium metal anodes employed for lithium metal batteries (LMBs). Structural and chemical defects are bad since highly defective graphene promotes unstable solid electrolyte interphase (SEI) growth. This consumes the FEC additive in the carbonate electrolyte and is correlated with rapid decay in CE and formation of filament-like Li dendrites. A unique flow-aided sonication exfoliation method is employed to synthesize “defect-free” graphene (df-G), allowing for a direct performance comparison with conventional reduced graphene oxide (r-GO). At cycle 1, the r-GO is better electrochemically wetted by Li than df-G, indicating that initially it is more lithiophilic. With cycling, the nucleation overpotential with r-GO becomes higher than with df-G, indicating less facile plating reactions. The df-G yields state-of-the-art electrochemical performance, with the post cycled metal surface being relatively smooth and dendrite-free. Conversely, r-GO templates have CE rapidly degrade from the onset, with extensive dendrites after cycling. We therefore propose the following design rule: An ideal architecture will promote copious heterogenous nucleation of the metal, shielding it from the electrolyte. However it is essential that the host is itself non-catalytic towards SEI formation.

2:00 PM

(GFMAT-095-2019) Interfacial reactions in sodium based batteries (Invited)

L. Ma[1]; R. Mogensen[1]; R. Younesi*[1]

1. Uppsala University, Chemistry-Ångström Laboratory, Sweden

The state-of-the-art batteries are almost exclusively based on lithium chemistry. Since the increased demand for batteries has put a pressure on raw material supply, rechargeable batteries based on abundant elements have become an important topic. Thus, sodium-ion batteries (SIBs) have recently attracted attention specially for applications where cost is a more important parameter than the energy density. Such batteries with energy densities of 300-350 Wh/kg (on an electrode level; 3-4 V cells) use non-aqueous electrolytes and low potential negative electrodes. Therefore, interfacial reactions in aforementioned batteries play key roles in order to make the batteries kinetically stable. The solid electrolyte interphase (SEI) is known as a passivation layer forms on the negative electrode via reduction of electrolyte components. In an ideal scenario, SEI forms during the initial discharge/charge with minimum consumption of charge, stays intact, and acts like as an efficient passivating layer which is ionically conductive and electronically insulating. SEI in SIBs have different properties than that in LIBs, mainly due to larger size, thus lower charge density, of Na^+ compared to Li^+. However, more research is needed to reveal details of SEI formation and its stability in SIBs. We have used different electrochemical techniques as well as spectroscopy methods to analyse composition of SEI and its dissolution rate in SIBs.

2:30 PM

(GFMAT-096-2019) Anode materials for Na-ion batteries and beyond (Invited)

A. Mukhopadhyay*[1]

1. Indian Institute of Technology (IIT) Bombay, Metallurgical Engineering and Materials Science, India

Limited and localized reserves of Li-precursors have necessitated looking beyond Li-ion batteries; with the Na-ion battery system emerging as a promising alternative. However, one of the major obstacles lies in the larger ionic radius and weaker ‘binding’ ability of Na^+ with graphitic carbon lattice. These render graphitic carbon not suitable as anode material for Na-ion batteries. Nevertheless, $Na_2Ti_3O_7$ is a potential anode material; which, however, lacks in terms of cyclic stability. In this context, some insights into the electrochemical reversibility of the same, as obtained via in-situ synchrotron XRD and Raman studies, will be presented here. These studies suggest that the formation of ‘impurity’ phase(s), and not instability/irreversibility of $Na_4Ti_3O_7$, is the major cause for capacity fade. Incorporation of carbon nanotubes could significantly improve the performance by maintaining connectivity, despite the formation of impurity phase(s). With respect to ‘alloying reaction’ based anode materials, our recent studies have indicated that electrochemical reversible Na-alloying is possible in Si, albeit with the performance depending strongly on the dimension and structure. This has established the potential of Si as an anode material for the Na-ion system. Lastly, some recent findings and understandings with respect to the usage of graphenic carbon as anode material for the upcoming K-ion battery system will be presented.

Li-ion Battery

Room: Salon D
Session Chair: Claude Delmas, Université Bordeaux

3:20 PM

(GFMAT-097-2019) Ion Dynamics in Solid-State Electrolytes and Electrodes as Revealed by Magnetic Resonance Imaging and Spectroscopy (Invited)

J. D. Bazak[1]; G. Goward*[1]
1. McMaster University, Canada

Our group have studied several Li+ conducting solid-state electrolyte and electrode materials, utilizing a range of magnetic-resonance strategies to compare and quantify ion transport processes. This talk will focus on our newest work in solid-electrolytes, which relies on ^{7}Li spectroscopy acquired at 20T magnetic field strength, paired with pulsed-field gradient diffusion measurements, acquired under ultrahigh gradient strengths. These methods reveal both the number of local environments involved in exchange, and the diffusion timescales, as a function of temperature. These methods, appropriate for solid-state electrolytes, are compared with our earlier work on in situ studies of concentration gradients in solution-state electrodes, and within graphite electrodes.

3:50 PM

(GFMAT-098-2019) Toward the development of aqueous batteries: Mastering the electrochemical interfaces (Invited)

A. Grimaud*[1]
1. College de France - CNRS, France

Since its first commercialization in the early 1990's, the Li-ion batteries (LIB) technology has spurred the spread of portable electronics as well as enabled the realization of electrical vehicles. Nevertheless, challenges still remain concerning the capacity of LIBs to enable the use of renewable energy to the grid while minimizing its footprint. Efforts have thus been made in developing sustainable electrode materials as well as electrolytes. Toward that goal, aqueous electrolytes could provide a lower-cost, safer and non-toxic alternative, providing that the overall battery performances are optimized for long-term application.
Started in 1994, the quest for aqueous batteries quickly showed limitations owing to their poor energy density limited by the narrow electrochemical stability window of water (1,23 V). Searching for new strategies in order to increase the electrochemical window of water is therefore crucial for the development of aqueous batteries. Adopting an electrocatalytic approach, the role of water solvation structure on its reduction occurring on the surface of negative electrodes will be discussed in this talk. The feasibility to completely suppress this reduction will be assessed and strategies consisting in using the reactivity of products formed upon water reduction for passivating negative electrodes will be proposed.

4:20 PM

(GFMAT-099-2019) Reversible oxygen-redox chemistry for large-capacity battery electrodes (Invited)

M. Okubo*[1]
1. University of Tokyo, Japan

Increasing the energy density of rechargeable batteries is of paramount importance toward achieving a sustainable society. The present limitation of the energy density is owing to the small capacity of cathode materials, in which the (de)intercalation of ions is charge-compensated by transition-metal redox reactions. Although additional oxygen-redox reactions of oxide cathodes have been recognized as an effective way to overcome this capacity limit, the electronic structure during oxygen-redox reactions are yet to be fully understood. In this work, we employed combined spectroscopic and theoretical electronic-structure analyses to demonstrate how reversible oxygen-redox reactions occurs in transition-metal oxides.

4:50 PM

(GFMAT-100-2019) Mxenes: 2D materials for high-performance batteries (Invited)

W. Luo*[1]
1. Uppsala University, Sweden

Transition metal carbides/nitrides (Mxenes) are an emerging class of 2D materials. Till date more than 20 Mxenes have been experimentally synthesized and the structure and properties of many more have been computationally predicted. The versatility in the chemistry of Mxenes and ease of tuning their properties has recently drawn a significant interest from a larger diaspora. The rationale for choosing these two candidate Mxenes is that carbide Mxenes (Ti_2C, Ti_2C_3 etc.) has been widely explored for battery applications whereas the nitride based Mxenes (for example Ti_2N) are rather recent additions. To be specific, V_2NS_2 and Ti_2NS_2 have been explored with a focus on computing meaningful descriptors to quantify these 2D materials to be optimally performing electrodes. The Li/Na ion adsorption energies are found to be high (>-2 eV) on both the surfaces and associated with significant charge transfer. Interestingly, this ion intercalation can reach up to multilayers which essentially affords higher specific capacity for the substrate. Particularly, these two 2D materials (V_2NS_2 and Ti_2NS_2) have been found to be more suitable for Li-ion batteries with estimated theoretical capacities of 2 99.52 $mAhg^{-1}$ and 308.28 $mAhg^{-1}$ respectively. Present examples can be viewed as a test case for future 2D material for anode applications.

Young Professionals Forum - Next Generation Materials for Multifunctional Applications and Sustainable Development, and Concurrent Societal Challenges in the New Millennium

Advances in Biomedical Science and Engineering II

Room: Trinity I
Session Chairs: Sahar Mahshid, Sunnybrook Research Institute; Daniele Benetti, Institut National de la Recherche Scientifique

8:30 AM

(YPF-008-2019) Nanosurface fluidic devices based on 2D and 3D nanostructures for optical and electrochemical detection (Invited)

S. Mahshid*[1]
1. McGill University, Bioengineering, Canada

Diagnostics of pathogenic and genetic disease (such as cancer) at the point of need, in particular at early-stage, requires dynamic manipulation and concentration of small number of target molecules at individual single-molecule level. In my lab, we focus on engineering new approaches in lab-on-chip technology via synergistically combining nanostructured materials with fluidic sample delivery systems with enhanced optical and electrochemical properties. Nanostructured materials boost the sensor resolution and show higher biochemical sensitivity and selectivity by significant amplification of the detection sites. We investigate fabrication of novel nanostructured platforms based on 3D materials such as gold and 2D materials such as graphene and molybdenum disulfide; integration of nanostructures with fluid sample delivery and biological assays; and implementation of the device for detection of small molecules, pathogens and cancer biomarkers. We address fundamental questions including: optimal interface of nanostructures with fluidic devices; target isolation, preparation and concentration in fluidic devices. We have successfully implemented the nanosurface fluidic devices for quantitative detection of Escherichia coli (E.coli) and Methicillin-resistant Staphylococcus aureus (MRSA), electrochemical detection of dopamine and optical detection of extracellular vesicles (EVs).

9:00 AM

(YPF-009-2019) Mechanical behavior of pva-h with fluid-solid mixture structure using mixing theory for nucleus pulposus replacement

M. Heo*[1]; C. Han[1]; C. Han[1]

1. Pusan National University, Republic of Korea

Polyvinyl Alcohol-Hydrogel (PVA-H) is well known a biomaterial used for manufacturing contact lenses as well as for the medium of drug delivery. Previous studies have also shown that PVA-H exhibits superior biocompatibility with hydrophilic elastic nature. The objective of this study was to determine the static and dynamic mechanical properties of PVA-H at different ratios of polyvinyl alcohol (PVA) and phosphate buffered saline (PVA) to determine the possible use of PVA-H as an alternative material to nucleus pulposus of the intervertebral disc. PVA-H specimens were made by changing the ratio of PVA, PBS and DMSO compositions (PVA-H1: 3 wt% PVA and 97 wt% PBS; PVA-H2: 5 wt% PVA and 95 wt% PBS; PVA-H3: 7 wt% PVA and 93 wt% PBS; PVA-H4: 10 wt% PVA, 90 wt% PBS. Unconfined and confined tests were carried out to measure the mechanical properties of PVA-H1, -H2, -H3 and -H4 within PBS solution. The mixture theory was applied to the results of unconfined and confined tests to investigate the mechanical properties reflecting the structural characteristics of fluid-solid mixture structure of nucleus pulposus in intervertebral disc. We used finite element analysis (FE-bio) with mixture theory to determine the composition of pva-h that is suitable to replace the intervertebral disc.

9:20 AM

(YPF-010-2019) From Nano to Micro – Synthesis and Optical Characterization of Rare-Earth-based Materials

E. Hemmer*[1]

1. University of Ottawa, Chemistry and Biomolecular Sciences, Canada

Based on their outstanding optical properties, Ln^{3+}-based compounds have been suggested for a wide range of applications including the fields of biomedicine, optoelectronics, and solar energy conversion. For instance, the capability of Ln^{3+}-based materials to emit visible and near-infrared (NIR) light under NIR excitation is highly sought after when aiming for biomedical applications. This is due to the fact that NIR light penetrates deeper into biological tissue when compared to UV or visible light. Fluorides of the general composition $MREF_4$ (M = alkali metal, RE = rare earth), are commonly considered as suitable host materials for upconverting and NIR emitting Ln^{3+} ions (e.g. Er^{3+}, Tm^{3+}, Ho^{3+}). The microwave-assisted approach offers a promising alternative for the synthesis of $MREF_4$ particles spanning the nano to micro scale. This presentation will shine a light on the versatile landscape of RE^{3+}-based materials focusing on materials synthesis and RE^{3+}-specific optical features.

9:40 AM

(YPF-011-2019) Strain engineering and surface hydrophobicity of NiTi shape memory alloys

P. Wu*[1]

1. Singapore University of Technology and Design, Entropic Interface Group, Engineering Product Development, Singapore

Hydrophobicity of solid surfaces depends on surface chemistry, strain and temperature. In particular, NiTi shape memory alloy undergoes phase transition in a wide range of strain-temperature conditions, which provides an additional parameter in the design of surface hydrophobicity of NiTi shape memory alloys. There is, however, neither adequate knowledge nor equation on how to calculate the water contact angles on NiTi films at specific surface strain and temperatures. Here we aim to establish a function of water contact angle with NiTi phase transition properties at various temperature-strain conditions. Our findings are useful for new practice in a wide range of research including antifouling applications. This study is an extension of our previous works; (1) an equation of water contact angle calculation from system entropy, (2) an equation of temperature dependent strain energy from system entropy, (3) dopant modulated crystal ductility, and super anticorrosion. We first derived a new equation to calculate water contact angles based on entropy at different strain, temperature, and surface roughness conditions. We, then, conducted experiments to calibrate the newly established equations. This research may provide novel insights on strain effects to crystal nucleation and crack propagation at nanoscale.

Advances in Thermoelectric Materials

Room: Trinity I

Session Chair: Tanmoy Maiti, Indian Institute of Technology Kanpur

10:30 AM

(YPF-012-2019) $SbSe_2$-based layered oxyselenides as a candidate multifunctional material for thermoelectric conversion and superconductivity (Invited)

Y. Goto*[1]; Y. Mizuguchi[1]

1. Tokyo Metropolitan University, Japan

Thermoelectric conversion is a promising approach that directly converts temperature difference into electricity. Recent first-principles calculations predicted that layered pnictogen oxychalcogenides $REOPnCh_2$ (RE = rare earth ion, Pn = pnictogen, Ch = chalcogen) as a high-performance thermoelectric material [M. Ochi et al. Phys. Rev. Appl. 8, 064020 (2017)]. This family of compounds has been extensively studied as a superconductor when Pn = Bi [Y. Mizuguchi, arXiv:1808.05782.], but the first-principles calculations showed that an increase of thermoelectric properties by substituting Bi with Sb. In the present study, we demonstrate the synthesis and thermoelectric properties of $REOSbSe_2$ [Y. Goto et al. J. Phys. Soc. Jpn. 87, 74703 (2018).]. Typical parent compound $LaOSbSe_2$ is an insulator with optical band gap of 1.0 eV. To obtain electrically conductive sample, we employed two approaches: (i) electron doping by substituting O^{2-} with F^-, and (ii) applying chemical pressure by substituting La with RE that has a smaller ionic radius [Y. Goto et al. J. Phys. Soc. Jpn. in press.]. Further, we prepared $RE(O,F)(Sb,Bi)Se_2$ solid solution to investigate the insulating $SbSe_2$- and superconducting $BiSe_2$-system. In the conference, we will also present our recent progress for emerging superconductivity in these compounds using ultra high-pressure technique.

11:00 AM

(YPF-013-2019) Generating thermoelectricity with flexible organic polymers (Invited)

E. Orgiu*[1]

1. Institut National de la Recherche Scientifique, Energy Materials Telecommunications, Canada

The quest for high-efficiency heat-to-electricity conversion has been one of the major driving forces toward renewable energy production for the future. In this context, the enhancement of the thermoelectric figure of merit $zT = \sigma S^2T/\kappa$ is imperative. Whilst there is already reported experimental evidence of zT~0.3 for organic semiconductors (OS) [1], the role of morphology and system dimensionality (2D vs. 3D) in determining zT is yet to be understood for OS. Unlike their inorganic counterpart, OS are held together by weak supramolecular interactions, therefore the way these materials are processed can lead to different molecular architectures [2]. In my talk, I will show how it is possible to realize different molecular architectures by playing with the deposition parameters of a conjugated polymer. In particular, seminal experiments will be presented that tackle the role of morphological anisotropy and dimensionality on the thermoelectric properties of such films. We use Langmuir-Schaefer technique to fabricate the films and vary the deposition parameters of the polymer solution, to change the surface polymer density and thickness, as well as the compactness and anisotropicity of the so-assembled nanofibrils. This study paves the way for the integration of our films in real organic-based thermoelectric devices, which currently only need a 3- to 4-fold increase to be technologically relevant.

Perovskites for Novel Applications

Room: Trinity I
Session Chair: Yosuke Goto, Tokyo Metropolitan University

1:30 PM

(YPF-014-2019) Micro-plasma based surface modificaiton and enhancement in dielectric and piezoelectric properties of ZnO and BaTiO3 based multifunctional composite thin films (Invited)

S. Banerjee*[1]; S. Ahmed[2]; E. Leal-Quiros[3]

1. California State University, Fresno, Mechanical Engineering, USA
2. State University of New York - Buffalo State, Mechanical Engineering, USA
3. University of California, Merced, Mechanical Engineering, USA

Atmospheric pressure and ambient temperature based micro-plasmas have been used in polarization and alignment of dipoles in ferroelectrics. The same phenomenon can be used to enhance the surface energy and surface characteristics of composite multifunctional thin films by means of surface modification. A significant increase in non-thermal atmospheric plasma applications, such as dielectric barrier discharge (DBD) and corona discharge plasmas have been steadily increasing in industry and in the research literature. The current work involves the use of corona discharge and DBD based micro-plasmas for surface modification of ZnO and BaTiO3 based multi-functional and flexible thin film devices towards enhancement in surface bonding characteristics and variation in surface wettability and surface energy characteristics. The parameters being investigated in the experiments include plasma device characteristics such as voltage, current, and frequency, as well as other significant parameters such as displacement between thin film and DBD/corona discharge source, treatment time, and temperature of the plasma. The modified surface micro-structure is analyzed using a scanning electron microscope and the bulk electrical and dielectric properties are characterized using impedance spectroscopy.

2:00 PM

(YPF-015-2019) Simulation studies of Viable Perovskite Photovoltaic Devices utilizing Non-toxic and Cheap Material Alternatives (Invited)

S. Ahmed*[1]; S. Banerjee[2]; S. Chowdhury[3]

1. State University of New York - Buffalo State, Mechanical Engineering, USA
2. California State University, Fresno, Mechanical Engineering, USA
3. Portland State University, Mechanical and Materials Engineering, USA

In this research, we have utilized simulation studies to probe non-toxic Sn and Sb-based perovskites with a goal to explore optimal fabrication methodologies. To that end, we have investigated a device structure with and without an electron transport layer - ETL - (both TiO_2 and ZnO have been explored) and assessed the impact on critical photovoltaic parameters. We have also explored Cu_2O as a viable hole transport layer (HTL) alternative to the traditional Spiro OMeTAD structure owing to ease of fabrication. Lastly, we have incorporated Cu as a viable back-contact alternative to the expensive Ag. We have performed optimization of individual layer thicknesses, thereby ultimately fabricating a device with the highest possible theoretical efficiency. The analyses provide critical insight into charge mobility and charge transfer kinetics within this non-Pb based device with cheap and easily fabricated materials; by observing the effects on Jsc, Vcc, and FF as individual layer thicknesses are modulated, and doing comparisons of structures with and without the various ETL layers, we present results of a structure that is not only optimal from an efficiency standpoint, but also from a technology viability and sustainability standpoint.

2:30 PM

(YPF-016-2019) Oxide Double Perovskites for High Temperature Thermoelectric Power Generation (Invited)

T. Maiti*[1]

1. Indian Institute of Technology Kanpur, Materials Science and Engineering, India

In this talk an overview will be presented on our recent work on double perovskites-based oxide thermoelectrics for clean energy generation by recycling waste heat produced in manufacturing industries, automobiles, power plants etc. Double perovskites were extensively investigated over the years for colossal magneto-resistance, ferroelectricity, high Tc superconductivity, multi-band Mott insulators etc. However, in the past 4 years, we have shown that oxide double-perovskites can be considered for high temperature thermoelectric power generation due to their environment-friendly nature, high-temperature stability, and lower processing cost compared to conventional chalcogenides and intermetallics. We have shown that decoupling of phonon-glass and electron-crystal behavior is possible in oxides by reducing thermal conductivity due to induced dipolar glassy state as a result of relaxor ferroelectricity. We have also introduced metal-like electrical conductivity ($\sim 10^5$S/m)in these ceramics that are inherently insulator in nature. Moreover, we have observed interesting behavior of temperature-driven p–n type conduction switch- ing assisted colossal change in thermopower in some of these oxides, hitherto, obtained only in chalcogenides. The charge transport mechanism in these complex oxides has been analyzed by small polaron hopping conduction model in conjugation with defect chemistry.

Design and Development of Novel Functional Materials

Room: Trinity I
Session Chairs: Akira Miura, Hokkaido University; Saquib Ahmed, State University of New York - Buffalo State

3:20 PM

(YPF-017-2019) Graphene: A multifunctional material to understand to design sustainable solutions (Invited)

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Graphene is a multifunctional material part of the solutions to reach sustainable development and societal challenges of the Millenium. This graphene-like material can be produced inspired by the principle of green chemistry, from clays and sugar, a renewable resource. The transformation of sugar into a graphene sheet is characterized using Raman and broadband dielectric spectroscopy, X-ray diffraction, thermogravimetric methods, X-ray photoelectron spectroscopy and transmission microscopy, which still remains challenging. For environmental application, this graphene hybrid porous materials can capture organic and inorganic pollutants. For health and energy transport application, graphene-polymer composites behave as dielectric materials. They have a percolation threshold according to the concentration and production method. The conductivity changes with the frequency and direction of the electric field. The material is anisotropic and the conductivity is greater in the longitudinal direction. The mechanical properties were tested in polymers with potential application for drones coating. Graphene-polymer composite had a greater toughness and strength, increasing with graphene concentration. For each application, the optimal concentration of graphene must be determined, to prevent waste according to green chemistry. Technology choices must keep in mind the Sustainable Development Goals.

3:50 PM

(YPF-018-2019) Viral design approach for 3D colloidal plasmonic nanostructures (Invited)

E. Sokullu*[1]; M. Pinsard[1]; J. Zhang[1]; J. Plathier[1]; G. Kolhatkar[1]; A. S. Blum[2]; F. Légaré[1]; A. Ruediger[1]; T. Ozaki[1]; M. A. Gauthier[1]

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The structure and properties of nanomaterials can be different for their ensembles compared to individual nanoparticles (NPs) and corresponding bulk materials. Self-assembly has emerged as a powerful technique to control these features and create well-defined nanostructures. In particular, ensembles of metallic NPs gain great attention as they are used to construct plasmonic nanostructures with enhanced optical properties. In this work, bacterial viruses, namely M13 and T4 phages, were used as biological templates to create well-defined gold aggregates with two distinct geometry, size, and plasmonic properties. Self-assembly was directed by displaying molecular recognition moieties on the phage surface which allowed control on the number of functional moieties at the genetic level. Thanks to the exceptional symmetry, mono-dispersed size and shape of the phages, gold NPs were deposited with precise interparticle distance. Their plasmonic properties were investigated by Surface enhanced Raman scattering and two photon induced fluorescence imaging. In both studies, the signals originated mainly from the surface of the gold NPs, within the interparticle nanogaps due to the plasmonic near-field enhancement. While both phage templates resulted in enhanced plasmonic properties, higher enhancements were observed with aggregates assembled on M13 phage which displays gold binding moieties with closer proximity.

4:20 PM

(YPF-019-2019) A Review on the Design of MAX and MAB Phase Reinforced Composites

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MAX Phases are novel ternary naturally nanolaminated carbides and nitrides. These novel solids have emerged as attractive candidate materials for multifunctional applications due to their interesting mechanical properties. Similarly, MAB phases are also novel ternary borides. Recently, there has been a renewed interest in MAB phases due to their mechanical properties which are intermediate between MAX Phases and binary borides. My research group is exploring these materials for usage as particulates in metal, ceramic, and polymer matrix composites. In this presentation, we will present some of the recent developments in the design of MAX phases reinforced composites.

Poster Session

Room: Salon A/B

6:30 PM

(BIO-P001-2019) Evaluation of Parenteral Glass Packaging with Multiscale Imaging Techniques

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1. US Food and Drug Administration, Center for Drug Evaluation and Research, USA

The existence of particulates in primary packaging results in potential risk for patients and costly product recalls. Here, we describe the evaluation of pharmaceutical glass containers for interaction with aqueous formulations using multiscale imaging techniques. We were able to detect heterogeneous alkali distribution using back-scattered electron imaging with scanning electron microscope (SEM), that enabled us to identify the most susceptible area at the inner vial surface. Comparison between non-treated as-received vials and vials with different formulations further revealed topographical changes under exposure to different aqueous solutions. Particulates that generated when exposed to aqueous formulations were filtered and characterized with digital microscope. The compositions of particulates were further analyzed with EDS, which would reveal the structure and explain the mechanistic of particulates generation. In this synergistic study, we explored glass heterogeneity under varied chemical conditions and its impact on pharmaceutical packaging. With the investigation of vials stored at various conditions, we found that high temperature and high pH can lead to glass degradation over a short period of time. Disclaimer: This article reflects the views of the author and should not be construed to represent FDA's views or policies.

(BIO-P002-2019) Large bone defect heal capacity of borosilicate bioactive scaffolds in goat tibia model

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2. Tongji University, School of Materials Science and Engineering, China

Repair of large bone defects caused by aging, traffic accidents and tumor resection are still facing a great challenge in clinical treatment. Borosilicate glass has excellent bone repair properties, and can form ion and alkaline microenvironment after degradation. By using the 3D printing technique and high temperature sintering method, high strength borosilicate bioactive scaffolds was fabricated. After immersed in PBS, the scaffold degraded and converted to hydroxyapatite, release the ions such as Ca^{2+}, Na^{+}, K^{+}, BO_3^{3-}, Si^{4+}, and create alkaline microenvironment. The ion and alkaline microenvironment can inhibit the bone resorption and stimulate the osteogenic differentiation and angiogenesis. After implanted in a goat tibia large bone defect, the scaffold did not cause local redness and inflammation, shows excellent biocompatibility. One week after surgery, the goats were able to walk around, and even jumped out of the sheepfold 2 months after surgery with a normal landing force for operated hind limb. At the same time, the scaffold can be degraded gradually in vivo and induce new bone and microvessels growth in, and ultimately achieve the restoring long-term mechanical stability and structural integrity of lager bone defect.

(BIO-P003-2019) Photothermal effect of graphene oxide-modified 3D-printed borosilicate bioglass scaffods

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1. Tongji University, School of Materials Science and Engineering, China

In recent years, photothermal therapy as a noninvasive, effective and low-toxic strategy to kill tumor cells has attracted considerable attentions. Furthermore, mild heat stimulation can also promote the healing of bone defects. Therefore, it is desired to combine both tissue engineering and photothermal therapy for bone cancer treatment, and simultaneously provide a scaffold for bone regrowth. For the purpose, we developed a bifunctional graphene oxide-modified borosilicate bioglass scaffold (GO-BG) by 3D-printing and surface-modification strategies. The GO-BG scaffolds exhibited excellent photothermal effects under the irradiation of 808 nm near infrared laser, and the photothermal temperatures could be modulated in the range of 40-80 °C by controlling the GO concentrations, surface-modification times and power densities of NIR. The photothermal effect of the GO-BG scaffolds induced more than 90% of cell death for osterosarcoma cells in vitro. Meanwhile, it is demonstrated the GO-BG scaffolds could promote the adhesion and differentiation of osteoblasts. The present study provides new insights into the design and fabrication of new-style osteoimplants.

(BIO-P004-2019) Physicochemical and biological properties of bone cement made from bioactive borosilicate glass containing strontium

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To determine the optimal strontium content in glass particles, a kind of novel bone cements composed of the bioactive borosilicate glass particles containing different amounts of Sr (0 to 12 mol% SrO) and the chitosan solution was made in this work. The injectability, setting time, compressive strength, degradation rate and bioactivity of these cements were evaluated in vitro. The ability of Sr ions released from the cements to modulate the proliferation, differentiation and mineralization of human bone marrow stem cells (hBMSCs) was studied in vitro. After comparing the physicochemical and biological properties, some of these cements were implanted for up to 8 weeks in a rabbit femoral condyle defect model in vivo and evaluated for their capacity to stimulate the healing of bone defects. The evaluation was arrived by the Van Gieson's picrofuchsin stain to identify new bone formation at the bone-cement interface. From the results of osteogenic capacity of this kind of bone cements, the work was concluded that the cement (designated 2B6Sr) composed of glass particles containing 6 mol % SrO content, supported better peri-implant bone formation and significantly higher bone-implant contact area than the cements containing 0 or 9 mol % SrO content.

(BIO-P005-2019) Angiogenesis and full-Thickness wound healing efficiency of a copper-doped borate bioactive glass/poly (lactic-co-glycolic acid) dressing loaded with vitamin E in vitro and in vivo

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Cu-doped borate bioactive glass (BG) microfibers have been proven to stimulate the proliferation of endothelial cells and upregulate VEGF gene expression. However, the release of effective ions is uncontrolled in the degradation process, leading to initially burst release, being toxic to the surrounding cells. To solve the problem, a composite dressing of Cu-doped BG microfibers and poly (lactic-co-glycolic acid) (PLGA) with various concentrations of vitamin E (VE) (VE-Cu BG/PLGA) was fabricated, in which PLGA is adopted as a substitute matrix for controlling the ion release rate of Cu-doped BG microfibers and VE was loaded because of its antioxidant and anti-inflammatory properties. In vitro results showed that the dressing was an ideal interface for the organic–inorganic mixture and a controlled release system for Cu^{2+} and vitamin E. Cell culture was suggested that the ionic dissolution product of the dressing improved the cell migration, tubule formation, and vascular endothelial growth factor (VEGF) secretion in human umbilical vein endothelial cells (HUVECs) and expression levels of angiogenesis-related genes in fibroblasts in vitro. These results indicate that the VE-Cu BG/PLGA dressing is a promising wound dressing in the reconstruction of full-thickness skin injury.

(BIO-P006-2019) Stereolithography of osteoconductive elastic bone implants based on hydrogel and octacalcium phosphate

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Most of the modern bone implants (metal alloys, ceramics and polymers) require additional surgery and their full or part replacement during the usage. Also it usually is challenging to fill and restore hard-to-get defects with a complex shape. This study aims at the creation of the material with the following properties: a) elasticity; b) biocompatibility and biodegradability, led to complete substitution of the implant by native bone tissue; c) osteoconductivity, i.e the permeability of the implant for bone tissue growth, blood vessels, nutrients etc. through interconnected macropores (of about 500-1000 μm). Such complex property set determined by choosing of polyethylene glycol diacrylate (PEGDA)-hydrogel as elastic matrix, layered calcium phosphates like brushite and octacalcium phosphate as inorganic filler and stereolithography (DLP) 3D-printing as the accurate way of formation of macroporous materials with specific architectures (Kelvin structure, gyroid- and diamond-types). For these biocomposites the composition of suspesion for DLP-printing was revealed, rheological, mechanical and toxicological tests were carried out and preliminary in vivo study on the model of monocortical rat defect was done. The work was supported by RSF, grant #17-79-20427. The authors acknowledge partial support from Lomonosov Moscow State University Program of Development.

(BIO-P007-2019) Resorbable ceramic materials based on calcium magnesium phosphates for bone regeneration

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An ideal material for regeneration of bone tissue in reconstructive and corrective surgery and orthopedics, needs to be porous in order to allow the growth of blood vessels, nerve tissue and bone cells proliferation. Such materials compensating for the lost area of bone tissue should create necessary conditions for its regeneration. In this study, we are obtaining porous resorbable ceramic materials based on calcium magnesium phosphates. According to the laser granulometry of calcium magnesium phosphate, the nanoparticle are suitable for 3D printing where they have a dark gray color, due to the presence of decomposition products of ammonium acetate. The resulting composite (monomers/powder) structures in the form of a Kelvin structure were exposed to a temperature of up to 1200°C. The study of the metabolic activity of cells in the presence of extracts from the material showed that the materials are able to support the adhesion, spreading and proliferative activity of human mesenchymal stem cells. These samples of biomaterials are biocompatible and do not have a cytotoxic effect on mammalian cells. The resulting ceramic materials are suitable for the creation of resorbable bone implants, including individually designed inorganics bases for the treatment of bone defects. Acknowledgement: This work was supported by the RFBR, grant nos. 18-29-11079, 18-53-00034.

(BIO-P008-2019) Effect of fluorapatite (FAp) coating on transform reaction of dicalcium phosphate dihydrate (DCPD) to FAp

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A dicalcium phosphate dihydrate (DCPD) transforms to more stable calcium phosphate such as hydroxyapatite (HAp) and fluorapatite (FAp). This reaction have been applied to serf-setting calcium phosphate cements. We previously appeared that the transform reaction of DCPD requires the formation "nano-surface structure" on surface of the DCPD particle. In this research, we investigated effect of coating of nano-scaled hydroxyapatite (HAp) and FAp nano-particle on surface of theDCPD particle by soaking the DCPD into an aqueous solutions. HAp precursor was successfully induced by using simulated body fluid (SBF), however the solution containing only calcium and phosphate ions (Ca-P solution) did not induce any precursor. FAp precursor was successfully induced by addition of fluoride ion in the Ca-P solution (Ca-P-F solution). More FAp precursor successfully induced by renewing the Ca-P-F solution every day and soaking DCPD for 3 days. The FAp-hybridized DCPD reacted fluoride ion with shorter induction periods that observe on reaction of DCPD and fluoride ion. The induction periods becomes shorter using FAp-hybrid induced by renewing the Ca-P-F solution every day. From these results, induction of FAp by using the Ca-P-F solution is applicable to improve reactivity of DCPD.

(BIO-P009-2019) 3D printed bioceramic microfluidic chip for biomimetic bone microenvironment and osteogenic drug screening

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Recently, microfluidic devices have been engineered to mimic tissues and organs to model the physiological cellular microenvironment. Organs-on-chips show great potential as alternatives for replacing animal testing for biomedical, pharmaceutical, and toxicological applications. As an important part of human body, bone plays a decisive role in the health of the human. Hence bone systems have been proposed as efficient three-dimensional (3D) in vitro models for studying complex biological phenomena in living systems. However, traditional microfluidic chip materials(such as silicon wafers, glass and PDMS) do not mimic the bone microenvironment well. Hydroxyapatite (HA) is the main inorganic component of bone, with biological activity, seems to be the better solution. In this study, we first proposed the use of hydroxyapatite as a microfluidic chip material that is highly biomimetic in bone environment, enabling high-throughput drug screening and exploring the interaction of bone cells with other cells. With the Stereo Lithography Appearance (SLA) technology, we designed and prepared many types of ceramic chips. We used a bioceramic chip to form a concentration gradient of DOX drugs, and determine the optimal concentration of the drug for osteosarcoma cell. This study provides a new strategy for the preparation of bone-on-a-chip and deserves further study.

(BIO-P010-2019) Evaluation of controlled cisplatin delivery in calcium phosphates/silicates nanoparticles for bone cancer therapy

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Bone cancer disease requires a novel anti-tumor loaded bone graft for specific delivery and regeneration of the structural defects after tumor resection. In this work we report about the drug delivery kinetics of bovine bone hydroxyapatite (BHAp) or silicocarnotite ($Ca_{5-x}(PO_4)_{2+x}(SiO_4)_{1-x}$;x≤0.3) spray dried spherical agglomerates of ceramic nanoparticles functionalized with cisplatin. The silicocarnotite phase was obtained from BHAp and a commercial bioactive glass by solid state reaction. The ceramic nanoparticles were obtained from high energy ball milling in a SPEX mixer/mill following an optimization procedure by 2^3factorial experiment design. The nanoparticles were characterized by X-ray diffraction and GSAS®Rietveld refinement to determine the crystallographic parameters of the correspondent phases such as crystallite size, unit cell volume, Ca/P ratio among others. The influence of morphology, size distribution and osteoconductive properties of spray dried spheres from both ceramics on the cisplatin adsorption/desorption kinetics was studied by UV-vis, in-vitro and degradation tests.

(BIO-P011-2019) Polypyrrole-coated poly(vinyl alcohol) fibers with improved neural performance at the tissue-electrode interface of brain implants

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For chronically implanted electrodes, tissue encapsulationcaused by cellular response and creation of fibrous glial encapsulation after implantation of many brain implants decreases the electrode efficiency due to poor electrode charge transfer ability. Surface characteristics at tissue-electrode interface play a key role in neural implant success. Surface modifications strategies involve multiple factors for desirableperformance of brain electrodes like high surface area, lowering electrode impedance, enhancing charge density, balancing mechanical interface properties between the soft tissue and hard electrode, improved target cell adhesion, stability, better recording and stimulating. In this study, pyrrole was polymerized on poly(vinyl alcohol) (PVA) nanofibers to form a conductive interface for the modification of brain implants. The polypyrrole coated PVA fibers showed a positive zeta potential value of 57.5 ± 5.46 mV. The in vitro DAPI nucleus staining showed a superior cell attachment. Furthermore, subcutaneous in vivo biocompatibility demonstrated no sign of inflammatory response. The electrochemical impedance analysis confirmed low impedance at different frequency regions. The polypyrrole-coated PVA interface showed appropriate stiffness, positive charge, high fibrous surface area, low impedance, and promoted neural cell adhesion as efficient physical and chemical factors for the improvement of neural implants at the interface of brain tissue and electrode.

(BIO-P012-2019) Nitric oxide releasing coatings for the prevention of biofilm formation

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Bacterial adhesion followed by biofilm formation at an implantation site can pose a significant health risk for patients with indwelling medical devices an implants. NO is a diatomic free radical produced endogenously an innate host antimicrobial response against viruses, bacteria, parasites and fungi. The study fabricates a range of nitric oxide (NO)-releasing silane and sol-gel coatings to prevent biofilm formation onto titanium, (poly(ethylene terephthalate) (PET) and silicone elastomer (SE)). N-diazeniumdiolate nitric oxide donors were formed at the secondary amine sites on the aminosilane molecules producing NO-releasing polymeric coatings. The NO payload and release were controlled by the aminosilane precursor. A sol-gel coating made up of an alkylsilane/aminosilane system was then used to increase the surface area and thereby the NO payload. The antibacterial efficacy of these coatings was tested using a laboratory strain of Staphyococcus Aureus and a clinical isolate of Pseudomonas aeruginosa (PA14). The silanised NO-releasing coatings were shown to have were shown to significantly reduce P. aeruginosa adhesion over 24 h with the efficacy being a function of the aminosilane modification and the underlying substrate. These NO-releasing polymers demonstrate the potential and utility of this facile coating technique for preventing biofilms for orthopaedic implants.

(BIO-P013-2019) Green machining of Alumina Dental Prosthesis: Root Implant, Crown and Bridge

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Machining of sintered alumina is known to cause surface micro-defects thereby decreasing the fatigue strength and the fracture toughness. This was the main cause of failure in all ceramic dental implants and crowns made of alumina which otherwise were aesthetic and biocompatible. Herein, we explored a plastic dough processing of densely loaded alumina dough with moderate viscosity for molding to near net shape or extruded to blanks for machining. Dried blanks were machined into implants, crowns, bridges by computer numerical control machining and subsequently sintered. Optimized dough viscosity was evident to be shear thinning behavior with viscosity value of 40 kPa.s at 1.25 s^{-1}. Homogeneous particle distribution of the green blanks and microstructure of sintered body were revealed by SEM microscopic analysis. The extruded-sintered blanks showed flexural strength of 336±25 MPa and Weibull modulus of 12.207 with 90% confidence interval that is highly reliable with the standards of conventional process. Shrinkage analysis of samples revealed ~27% volumetric change with isotropic nature. Hence this novel processing route would be feasible for producing complete dental prosthesis including, customized root implant, abutment and crown.

(BIO-P014-2019) Cermet of Alumina - Ti_6Al_4V and green Machining

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Ceramic and metal composites are highly beneficial in high-temperature structural and functional applications as well as biomedical applications. Ceramics like alumina have high surface hardness, wear resistance and high temperature strength, but they are brittle, poor conductors of heat and electricity. By incorporating metallic phase like titanium, these functional properties can be achieved and fracture toughness and tribology of the resultant composite can be improved. However, their applications were limited due to high cost of sintering by SPS and difficulty in shaping. Herein, we explored a green machining process where the constituent powders of Ti6Al4V and alumina were made into a highly loaded homogeneous mixture with a polymer binder. The green body was extruded into blanks, dried, CNC machined and subjected to pressure less sintering under argon atmosphere at 1400 °C. Sample had good surface finish with retaining the details of machined features. μCT evaluation in green and sintered state showed homogenous particle size distribution with insignificant internal pores. XRD analysis revealed no appearance of any new phases. SEM and EDX analysis showed distinct grain boundaries with alumina grain interlocking in the titanium alloy matrix. Hence this novel processing route can be successfully applied as a cost effective alternate, for processing Cermets into complex shaped components including biomedical implants.

(BIO-P015-2019) Bioactive glass-containing coating layers on the surface of dental implants: An innovative approach to enhance bone regeneration at implant interface

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There have been several reports on the weak integration of metallic dental implants with the natural bone tissues. As an alternative, mesoporous bioactive glass materials can be used to enhance bone bonding ability upon implantation. In this research, bioactive glass added to zirconium titanate to produce a nanocomposite thin film on the surface of the dental implants applied via a sol-gel spin coating technique. The result showed a uniform layer on the surface of bioactive glass-containing coated dental implants through the optimization with carboxymethyl cellulose as dispersing agent. The biomineralization capability of the bioactive glass-containing coated dental implantsconfirmed the sustained release of calcium and phosphorous in the surrounding media, that further resulted a bone-like apatite layer on the surface of the implants. The bioactive glass-containing layers not only protected the surface of dental implants against corrosion and wear, but also advantageously enhance bone bonding ability upon implantation due to presence of biologically active bone-like apatite layers which acted as an interface enabling a strong bonding with the natural bone tissues.

(BIO-P016-2019) Bone Tissue Compatibility of Hydroxyapatite-coated PEEK with Foamed Surface

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Polyetheretherketone (PEEK) is used in orthopedics. However, PEEK is bio-inert material, and its fixation to bone is limited. We developed Hydroxyapatite-coated PEEK with foamed surface by novel technique. The aim of this study is to investigate the ability for fixation to bone by tissue integration. 3 kinds of samples (solid PEEK (SP), PEEK with foamed surface (FSP), and hydroxyapatite-coated FSP (HFSP)) were implanted to rabbit femoral bone. After 4 weeks and 12 weeks from implantation, biomechanical testing (push-out), histological analysis, and computed tomography (CT) analysis were carried out. The samples used in histological and CT analysis had a non-cylindrical shape on the assumption of application to jagged shape implant such as spinal cage. The push-out testing data showed that the shear strength of FSP was higher than that of SP at 4 weeks and 12 weeks after implantation, and these results indicated that surface porous structure contributed to fixation to bone. Histological study and CT analysis showed bone ingrowth even into pores of recess parts especially on HFSP. Hydroxyapatite coating promoted compatibility with bone tissue. In vivo study revealed HFSP's ability for fixation to bone by tissue integration. It is suggested that this material is useful for orthopedic implants which should be fixed to bone.

(BIO-P017-2019) A New Injectable Bone Graft Substitutes for Segmental/Large Bone Defects

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Purpose: Calcium phosphate cements have limitations such as mechanical weak, burst drug release and poor washout resistance. In this study, we described a new injectable polymeric brushite bone cements (P-DCPD) that is mechanical strong and capable of sustained antibiotics release. Methods: P-DCPD was prepared by mixing CPP gel with tetracalcium phosphate (TTCP). The physiochemical properties of P-DCPD was measured by FTIR and XRD. The cement setting mechanisms were investigated by AFM and Raman spectroscopy. The handling properties of P-DCPD (setting time, setting temperature, injectability, mechanical strength, viscosity and washout resistance) were investigated. Results: We compared the handling properties of P-DCPD with commercial Hydroset cements (Stryker). P-DCPD is superior to existing CPCs including, but not limited to, a constant viscosity, controllable setting, injectability and sustained drug release. An excellent washout resistance of P-DCPD was observed. This might be due to its high viscosity, short setting time (5-8 min) and the microstructure of entangled polyphosphate chains. A sustained release of vancomycin from P-DCPD for 2 months was observed. This might be due to the ionic interaction between vancomycin and the polyphosphate chains. Conclusions: We described a new way to prepare P-DCPD cement that can be used as a new bone void filler for the load-bearing and large bone defects.

(BIO-P018-2019) Immune response with nanorod-structured biphasic calcium phosphate ceramics and the regulation on MC3T3-E1 cells

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After implanted, the morphology of scaffolds will make an important effect on biological events. As been reported, it had a great contribution to immune response, including signal molecules secretion which play a decisive role in subsequent repair process. In this study, we used macrophages and MC3T3 as the cell models. Biphasic calcium phosphate (BCP) ceramics with different morphologies were used to investigate the immune response and their effect on osteogenesis. BCP were fabricated by H_2O_2 foaming method, and the surface covered with regular nanorod and irregular hollow nanorod were fabricated via different hydrothermal treatment subsequently. Western Blot and qRT-PCR were used mainly to evaluate the phenotypic polarization of macrophages and osteogenic differentiation of MC3T3. Besides, signaling pathway analysis was conducted to reveal the mechanism of surface morphology mediated crosstalk between inflammation and osteogenic differentiation. The result indicated that BCP ceramics with diverse morphologies have different stimulation on macrophages to secrete inflammatory molecules. The secreted TNF-a can make a contribution to the osteogenic differentiation of MC3T3-E1 cells on a dose-dependent pattern. High concentration of TNF-a have an inhibition on osteogenic differentiation via initiating NF-κB signaling pathway.

(BIO-P019-2019) Evaluation of durability of low temperature degradation free Zirconia toughened alumina head

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Zirconia toughened alumina (ZTA) are developed and has become mainstream of artificial hip joint alternative to alumina and zirconia. Although improvement of the mechanical characteristics of ZTA have been focused, surface changes in ceramic component under friction environment has not been clarified yet. Purpose of this study is to evaluate the interface of between ceramic head and other parts under severe condition. Low temperature degradation ZTA with 19 wt% zirconia was used for this study. Each three alumina heads, ZTA heads and metal heads were prepared for hip wear simulator study. Cross linked polyethylene (CLPE) liner was used as counter parts. Changes in weight loss of CLPE liner and surface morphology of heads during wear tests were evaluated. In the case of ceramic head, unlike in the case of metal heads, there were no remarkable adhesion of metal ion on the crevice region the taper trunnion after hip wear simulator test. There were also no significant changes in morphologies of surface of ZTA heads. However some shallow dents which were similar shape as alumina grains were observed on surface of alumina heads. These results support the results of previous studies on retrieved alumina head and hip simulator study using aged zirconia head. It is necessary to evaluate in detail about the surface changes under severe conditions and compare it with the clinical results.

(BIO-P020-2019) Evaluating the Platelet Activation Related to the Degradation of Biomaterials by Scheme of Molecular Markers

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The evaluation of platelet activation of medical devices using in cardiovascular system is very meaningful. Currently, it is mainly based on the ISO10993-4 international standard. However, the methods given in the standard are originally designed for non-degradable materials, the applicability, the operability, and the convenience to degradable materials of the methods needs to be carefully studied. In this study, the platelet activation by 3 typical degradable materials (collagen, polylactic acid and hydroxyapatite) were evaluated by three widely used molecular markers CD62P, CD63, CD40L and the three molecular markers PF4, β-TG and TXB2 mentioned in the ISO10993-4 standard. The variations of the six markers in a simulated degradation process of the degradable materials were compared. It was found that the degree of platelet activation changed with the degradation and was strongly relative with the surface physicochemical properties. For example, when the surface roughness and contact angle of the materials change, the degree of platelet activation also changes. These six platelet activation molecular markers can to be the promising key for the assessing of platelet function in degradable medical devices which is instructive for the quality control and the development of new degradable medical devices.

(BIO-P021-2019) Osteoinductivity of porous biphasic calcium phosphate ceramic spheres with nanocrystalline and their efficacy in guiding bone regeneration

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Conventional biphasic calcium phosphate (BCP) bioceramics are facing many challenges to meet the demands of regenerative medicine, their biological properties are limited to a large extent due to the large grain size in comparison with nanocrystalline of natural bone mineral. Herein, this study aimed to fabricate porous BCP ceramic spheres with nanocrystalline (BCP-N) by combining alginate gelatinizing with microwave hybrid sintering methods, and investigated their in vitro and in vivo combinational osteogenesis potential. For comparison, spherical BCP granules with microcrystalline (BCP-G) and commercially irregular BCP granules (BAM®, BCP-I) were selected as control. BCP-N with specific nanotopography could well initiate and regulate in vitro biological responds, such as degradation, protein adsorption, bone-like apatite formation, cell behaviors and osteogenic differentiation. In vivo canine intramuscular implantation and rabbit mandible critical-sized bone defect repair further confirmed that nanotopography in BCP-N might be responsible for the stronger osteoinductivity and bone regenerative ability than BCP-G and BCP-I. Collectedly BCP-N has excellent efficacy in guiding bone regeneration, and hold great potential to become a potential alternative to standard bone grafts in bone defect filling applications.

(BIO-P022-2019) Application of CaP biomaterials in repair of load-bearing bone defects

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Porous CaP ceramics were fabricated by a slurry foaming method, followed by a special hydrothermal treatment to make the scaffold skeleton transforming into HA whiskers, and further impregnated by vacuum a layer of nHA into the skeleton and calcined to further improve the mechanical strength of the scaffolds. The critical sized segmental bone defects were constructed in the femur of beagle and the skull of rhesus, respectively. The cylindrical and quadrate implants were respectively fixed into the defect sites. After 3 and 6 months of implantation, the bone repair in the defect sites were evaluated by micro-CT, histological analysis and biomechanical test. The CaP ceramics showed the significantly enhanced mechanical strength, and the in vitro cell study confirmed that the surface nHA coating endowed the ceramic with higher ability to promote the osteoblastic differentiation of MSCs than original ceramic. When used in both animal models, the osteoinductive CaP implants exhibited good repairing effect. A large amount of new bones formed in the inner pores of the ceramics, and the biomechanical strength of the defect sites was over 50% of natural bone. This study indicated

the good potential of the CaP ceramics in the load-bearing bone defect repair.

(BIO-P023-2019) Fracture Behavior and Stress Distribution of Monolithic and CAD/CAM Veneered Zirconia FDPs

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The purpose of this study was to evaluate the effect of 3-unit zirconia fixed dental prostheses (FDPs) design (monolithic vs. bi-layered) on fatigue life and the stress distribution under simulated chewing force using finite element analysis (FEA). Identical epoxy resin replicas of the mandibular second premolar and second molar were divided into four groups (n=10): thirty zirconia Y-TZP frameworks veneered by hand-layering technique (ZL), heat-pressing technique (ZP), and CAD/CAM technique (CAD-on), and ten monolithic zirconia FDPs (MZ). Specimens were subjected to compressive cyclic loading in a universal testing machine. Data was statistically analyzed with the Chi-square test and Kaplan Meier survival analysis (α=0.5). 3D models were constructed to analyze the stresses within the zirconia FDPs geometries using FEA. Specimens from the ZL and ZP groups exhibited failures at different stages during the fatigue test, while the CAD-on and MZ 3-unit FDPs survived with no failure. The Chi-square test showed a significant difference between the groups ($P<0.001$). The maximum principal stresses were located under the mesial connector in monolithic and bi-layered zirconia FDPs. These stresses were higher in monolithic geometries than bi-layered ones.

(YPF-P024-2019) Double perovskite based composite material for solid oxide fuel cell electrode application

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Composites materials have shown good ionic and electronic conductivity and usually called mixed ionic electronic conductor (MIEC). In the current investigation, we have synthesized the STC/3YSZ composite by using solid state reaction route for the solid oxide fuel cell (SOFC) electrode application. STC and 3YSZ powders have mixed in 1:1 ratio. XRD pattern analysis has confirmed composite phase formation while FESEM study illustrates a compact microstructure with little porosity. The apparent porosity is beneficial for the SOFC electrode because it provides path to flow of the gaseous species. Impedance spectra results follow the diffused semicircle which confirms the grain and grain boundary polarisation. Further, we analyzed the impedance data in ZView software using R-Q circuit and calculated different parameters like modulus, admittance and activation energy. The activation energy for STC/3YSZ composite material is found to be 0.71eV and 0.51 eV for grain and grain boundary respectively. It suggests that the conduction of carriers through grain boundary is easier comparison with grain.

(GFMAT-P025-2019) Band-gap energies and Seebeck coefficient of $Cu_2Sn(S_X,Se_{1-X})_3$ solid solution

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Cu_2SnSe_3(CTSe) is considered to be a promising thermoelectric (TE) material for replacing current commercial TE materials due to similar electrical/thermal properties and cheap/nontoxic elements. But ZT of CTSe is not comparable with those of PbTe and Bi_2Te_3 due to its low Seebeck coefficient. Making composites of CTSe with a TE material with large Seebeck coefficient such as SnS, can be one way to control its Seebeck coefficient, but the electrical conductivity of the parent CTSe can be largely compromised. Here we introduce a strategy to control Seebeck coefficient without losing large part of electrical conductivity of CTSe by making its solid solution with Cu2SnS3(CTS). Suppressing Se vacancies by introducing S in CTSe lattice can be used to control Seebeck coefficient. The analogous crystal and band structure of CTSe and CTS was the motivation behind the study of TE properties of $Cu_2Sn(S_X,Se_{1-X})_3$(CTSSe) ($0\leq X \leq 0.8$) solid solution. CTSe and CTSSe were prepared using mechanical alloying followed by spark plasma sintering. Rietveld refinements of powder XRD data were used to determine the variation of lattice constants of CTSSe with gradual replacing of Se with S. Here we report that the control of band gap and TE properties as well as the decrease of thermal conductivity can be efficiently achieved by optimization of the composition of CTSSe which can lead to enhanced TE performance of the CTSe.

(GFMAT-P026-2019) Densification and grain growth in alumina ceramics prepared via conventional sintering and spark plasma sintering (SPS)

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Ceramic processing is frequently confronted with the problem of finding an approriate compromise between densification and grain growth, which usually occur simultaneously. Since densification improves mechanical strength and grain growth tends to deteriorate it, it is essential to find a reasonable optimum between these two counteracting phenomena or to attempt to suppress grain growth, e.g. using advanced sintering techniques. In this work we compare the densification and grain growth of alumina ceramics prepared via conventional sintering and spark plasma sintering (SPS), also called electric current assisted sintering (ECAS). The bulk density (and open porosity) of partially sintered and fully dense alumina ceramics is determined via the Archimedes method, the grain size (mean chord length and Jeffries size) via stereology-based image analysis using global metric descriptors, i.e. interface density and mean curvature integral density (and total porosity via the Delesse-Rosiwal law). Shrinkage is measured after sintering as well as monitored in situ via dilatometry and SPS piston displacement. Also dihedral angles are measured and the grain size distributions are approximately reconstructed and analyzed. The results are discussed in the context of current grain growth theories and the concept of master sintering curves.

(GFMAT-P027-2019) The potential of brewery waste for the synthesis of Carbon Quantum Dot

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Brewery waste is formed in large quantities during beer fermentation. Its biodegradability property creates several alternatives for its valorization. We propose here an alternative method to reduce waste and add value to beer production by exploiting this rich carbon source and use it as a raw material for producing carbon quantum dots (CQD). CQD are known as small carbon nanoparticles with size lower than 10 nm. Their structure is characterized by multiple functional groups like hydroxyl and carboxyl and a sp^2 conjugated core. Their various properties, in particular their high photoluminescence and their low toxicity, give them a certain notoriety within the multiple quantum dot. Several studies also highlight the synthesis of CQD from biosources, various methods of synthesis have also been explored. However, very few studies demonstrate that the CQD can be synthesized by microwave radiation with breweries waste as a precursor, hence the interest of focusing on the issue. The purpose of this document is to study the potential of brewery waste based CQD to act as sensors for metal ions detection which represents a real source of pollution above a certain threshold. We have to present a complete synthesis method using microwave radiation. To characterize the CQD, UV-Vis, fluorescence and FTIR spectroscopy have been done. The Fluorescence Quenching Principle has been used for metal detection.

(GFMAT-P028-2019) Enhanced Thermoelectric Figure of Merit ZT In Halide Doped Bismuth Sulfide

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Over the past few decades, semiconducting chalcogenides compounds have been receiving much attention because of their wide range of applications in the various field of science and technology. The sulphides based metal chalcogenides (Bi_2S_3, $Cu_{2-x}S$, CdS, TiS_2, Ag_2S etc.)as TE materials find a high interest in research field due to their low cost, low toxicity, more abundant and optimisable TE property. Besides these advantage sulfides have some challenges such as its volatility, poor transport property which limits the TE performance. Various strategies have been used for improving its TE performance such as doping etc. Here we report the synthesis and thermoelectric properties of SPSed Bi_2S_3 doped with x- mole% $CuCl_2$. Powder of stoichiometric compositions was prepared by melt and growth process inside a quartz evacuated tube. First, we ground the as-synthesized ingots and sintered by SPS. XRD of all the samples showed single phase formation. SEM analysis of these materials demonstrated the plate-like morphology indicating that these crystals were grown layer by layer mechanism. All the compositions showed a negative Seebeck coefficient suggesting n-type behavior. The decrease in band gap observed with increasing dopant concentration lead to the improvement in its electrical property resulting higher power factor ~2000 $\mu W/m\text{-}K^2$. ZT value greater than 1 was achieved in these halide doped chalcogenides.

(GFMAT-P029-2019) Synthesis of molybdenum trioxide nanoparticles by pulsed wire discharge using multiple molybdenum wires

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Molybdenum trioxide is used in industry as catalysts, electrical-electronics devices, and recently its nanostructured materials draw interests. Especially from MoO_3 to synthesize ^{99}Mo by a nuclear reaction of ^{98}Mo, it could be the best solution to produce ^{99m}Tc for medical applications without using fission products. Therefore the nanoparticles of MoO_3 is required to make high-density pellets of MoO_3. The purpose of this research is to synthesize nanoparticles of MoO_3 by pulse wire discharge (PWD) with multiple molybdenum wires placed inside the chamber. From X-ray diffraction and scanning electron microscopy, nanoparticles of a single phase MoO_3 were successfully synthesized.

(GFMAT-P030-2019) Corrosion and Corrosion-Erosion resistance of Ni-Co -TiO2 nanocomposite coatings

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In the present work, TiO2 nanoparticles were synthesized by sol-gel method using titanium tetraisopropoxide as a precursor. Synthesized TiO2 nanoparticles were suspended in Ni-Co electrolyte and deposited with constant current density. The deposition was carried out for 30 minutes on a steel substrate with varying concentrations of TiO2 nanoparticles in Ni-Co matrix. The hardness values were found to be uniform on the coating and increases with the weight fraction of TiO2 nanoparticles. Average hardness of the steel substrate was found to be 184 HV and that of Ni-Co and Ni-Co-TiO2 coating were around 375 HV and 540 HV, respectively. SEM examination reveals that the co-deposited TiO2 nanoparticles were uniformly distributed and well bonded with the Ni–Co matrix. X-ray diffraction analysis confirmed that the electrodeposited Ni–Co alloy coating is composed of a solid solution and there is a decrease in grain size in the Ni-Co matrix. The latter is attributed to the addition of nano titania which creates more nucleation sites retarding the growth of the Ni-Co grains. Significant enhancements in the corrosion and erosion-corrosion resistance were obtained which is attributed to the presence of nano TiO2 particles coated under optimal electrodeposition conditions.

(GFMAT-P031-2019) Improvement of fatigue strength of thermoplastic composites reinforced by kenaf natural fibre

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Kenaf fibre reinforced polypropylene composites have found applications in construction and automotive industries. The fibre was subjected to an alkali-silane treatment to enhance the interfacial adhesion between the fibre and polypropylene matrix. The effect of this treatment on the fatigue strength of kenaf fibre reinforced polypropylene composites is investigated. Test results showed that fibre treatment consistently improves the fatigue strength of the composite. For instance, the fatigue performance of the alkali-silane treated kenaf/PP composite with 30% fibre loading is almost 100% higher than that of the untreated kenaf/PP composite. Microscopy examination revealed that failure mechanism of alkali-silane treated keanf/PP composites occurs in three phases, namely crack initiation, crack propagation followed by ultimate failure. Micro-cracks initiate predominantly in the matrix rather than in fibre-dominated regions. As the number of cycles increases, cracks propagate toward the fibre dominated-regions, mostly along the fibre-matrix interface, and the residual load-bearing capability of the composite drastically drops. Rapid spread of cracks takes place and this subsequently leads to fibre breakage.

(GFMAT-P032-2019) Effect of impurities on properties of calcium phosphates from unused phosphate and calcium resources

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Hydroxyapatite (HAp) adsorbs various gaseous chemical substances such as VOC (volatile organic compound) and ammonia. In addition, some reports described that metal ion-containing HAp has enhanced adsorption properties. In this study, we focused on the characteristics of metal-containing HAp and investigated synthesis of HAp from unused phosphorus and calcium resources for ammonia adsorbent. We selected sewage sludge as phosphorus resource. In case of phosphate recovery from the sewage sludge by acid extraction, obtained leachate contains metal ions such as iron and aluminum. We studied influence of the metal ions on adsorption performance for ammonia. HAp was precipitated by mixing calcium hydroxide and simulated extract from the sewage sludge. As a result, we found that aluminum and iron ions contained in obtained HAp and these metal ions improve the ammonia adsorption capacity of HAp.

(GFMAT-P033-2019) Reactivity improvement of dicalcium phosphate dihydrate (DCPD) with fluoride ion by using unused calcium resources

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Fluoride pollution in the water environments such as groundwater is one of the important environmental problems because fluoride affects human health and cause of dental fluorosis. From this background, removal of fluoride from the water environments have been widely required. Dicalcium phosphate dihydrate (DCPD) reacts with small amounts of fluoride ions in an aqueous solution and forms stable fluorapatite (FAp). In this study, we shows application of various unused calcium resources to produce removal agent for fluoride. We focus to DCPD of byproduct from gelatin production. We appeared that addition of calcium carbonate improve removal efficiency and inhibit release of phosphate ions of the DCPD reaction. We also appeared that sediment in Tunisian reservoir containing calcium carbonate. By using the DCPD-sediment mixture, fluoride ion in an aqueous solution was efficiently removed. From these results, utilize of sediment containing calcium carbonate is applicable to removal of fluoride in the water environments.

(GFMAT-P034-2019) Fabrication of textured B_4C with oriented pores via magnetic field assisted colloidal processing

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Boron carbide (B_4C) ceramics used as a neutron absorber in fast reactors get broken easily during operation because of volume swelling due to the accommodation of helium gas meanwhile the neutron absorption reaction. Releasing the accumulated helium is difficult because a conventional sinetered B_4C has only porosity of 5-10% without specific direction. However, helium release should be achieved in similar porosity to maintain the mechanical properties and the neutron-absorbing capability. In this study, to develop the B_4C neutron absorber with a longer lifespan than the current one, the conditions of the strong magnetic field-assisted colloidal process were optimized for fabricating the textured B4C ceramic with oriented pores. B_4C slurries including nylon 66, Al_2O_3 and CNT were consolidated by slip-casting on a turntable placed at a magnetic field of 12T. After burning off the nylon 66 and densifying by Spark Plasma Sintering, the textured B_4C with oriented pores can be obtained. Vertically oriented pores formed by burning off nylon 66 were found from SEM observation and X-ray Computed Tomography. Besides, horizontal alignment of the CNT in the B_4C matrix phase was indicated from the SEM observation and XRD analysis.

(GFMAT-P035-2019) Synthesis of ordered mesoporous silica from rice husk for recycling bioresource

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This study will present the synthesis of ordered mesoporous silica particles from rice husk by combining acid leaching, chemical dissolution and self-assembly with additional surfactants. High purity (99.8 wt%) silica is easily prepared by the acid treatment of rich husk, followed by the pyrolysis. The obtained silica powder was dissolved at alkaline solution to make sodium silicate that used as precursor. Mesoporous silica is synthesized by cooperative self-assembly process by employing additional surfactants with sodium silicate solution. Depending on the type of surfactant and the self-assembly condition, various ordered mesoporous silica which have 3 to 30 nm mesopores with high surface area are successfully synthesized. We expect the synthesis of high value-added silica by using abundant bioresource to open up new avenues for sustainable and environmental-friendly industrial development.

(GFMAT-P036-2019) Evaluation of $LiGaO_2$ single crystal scintillator for neutron detection

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In this study, we focus $LiAlO_2$ and $LiGaO_2$ scintillating crystals for neutron detectors since they contain Li in the chemical composition. In these crystals, thermal neutron can be measured in pulse height spectrum with clear neutron peak. Up to now, in inorganic scintillators, PSD can be possible in emission center doped materials, such as Ce-doped elpasolite and $LiCaAlF_6$ by using the intrinsic and extrinsic luminescence. In $LiAlO_2$ and $LiGaO_2$, we observed PSD properties in these crystals. To our knowledge, PSD in undoped materials is not common, and this work opens a new possibility to develop scintillators with PSD function.

(GFMAT-P037-2019) Evaluation of terbium activated $Sr_2(Y,Gd,Lu)_8(SiO_4)_6O_2$ single crystals on scintillation properties

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In the present study, we focus on the Tb-doped Sr-based apatite materials which have a chemical composition of $Sr_2RE_8(SiO_4)_6O_2$ (RE = rare earth element). Up to now, we have investigated Ce-doped apatite scintillators, and there still remains a large room for study for other emission centers. Tb 0.5% doped $Sr_2Gd_8(SiO_4)_6O_2$, $Sr_2Y_8(SiO_4)_6O_2$, $Sr_2(Gd_{0.5}Lu_{0.5})_8(SiO_4)_6O_2$ and $Sr_2(Gd_{0.4}Lu_{0.6})_8(SiO_4)_6O_2$ crystals were synthesized by the floating zone method. When we checked powder X-ray diffraction patter, we confirmed a single phase (JCPDS No:28-0212). In photoluminescence (PL) and X-ray induced scintillation spectra, some sharp emission lines appeared, and the emission origin was Tb_{3+} 4f-4f transition. We investigated PL and scintillation decay time profiles, and the main component was 1.8 and 1.3 ms, respectively. Among the samples prepared here, $Sr_2Gd_8(SiO_4)_6O_2$ showed the highest scintillation intensity.

(GFMAT-P038-2019) Fabrication of $Sr_{0.5}Ba_{0.5}Nb_2O_6$ Nanocrystallite-Precipitated Transparent Glass-Ceramics

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Transparent $(Sr_{0.5}Ba_{0.5})Nb_2O_6$ (SBN50) nanocrystallite-precipitated phosphate glass-ceramics were prepared by a conventional glass-ceramic process. x(SrO-BaO-2Nb_2O_5)-(100-4x)P_2O_5 (xSBNP) glasses with a refractive index of 1.9–2.0 exhibited high water resistance owing to the presence of Q^0 and Q^1 phosphate units. Both bulk and surface crystallization of the SBN50 phase were observed in 20SBNP and 21SBNP glass-ceramics. Although the nominal content of SBN50 crystals in the 21SBNP glass was larger than that in the 20SBNP glass, the latter exhibited better crystallinity of SBN50 and a higher number density of precipitated SBN nanocrystallites. By tuning the two-step heat-treatment and the chemical composition, transparent SBN50-precipitated glass-ceramics were successfully obtained. Given that no remarkable increase of the relative dielectric constants was observed after crystallization of the SBN50 nanocrystallites, it is postulated that the relative dielectric constant of the bulk is mainly governed by the amorphous phosphate region, and that the contribution of precipitation of the SBN50 nanocrystallites to the dielectric constant is not very significant in this system.

(GFMAT-P039-2019) Nano-phase separation and the effect of SnO addition in TiO_2-precipitated glass–ceramics

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We have investigated the nano-structure of TiO_2-precipitated CaO-B_2O_3-Bi_2O_3-Al_2O_3-TiO_2 (CaBBAT) glass–ceramics, and discussed the effect of the addition of SnO.^{119}Sn Mössbauer spectra of the Sn-doped glass suggest that most of the SnO was oxidized during melting. Selective crystallization of TiO_2 occurred independently of SnO addition in the homogeneous glass. However, EDX analysis of the glass–ceramics revealed that the Ti cation is partially localized and that the addition of SnO promotes the nano-phase separation. It can be concluded, therefore, that the addition of SnO influenced the formation of secondary particles of TiO_2 nano-crystallites and thereby improved the photocatalytic activity.

(GFMAT-P040-2019) Radiation response properties of strontium aluminoborate glasses doped with Ce

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Strontium aluminoborate glasses with different concentrations of Ce (0, 0.01, 0.05, 0.1 and 0.5 mol.%) were synthesized by the conventional melt-quenching technique. After the synthesis, photoluminescence (PL), scintillation and dosimetric properties of the samples were evaluated systematically. In the PL and scintillation spectra, a sharp peak at around 370 nm due to the 5d-4f transitions of Ce was observed. The 0.05% Ce-doped sample showed the highest intensity in PL and scintillation among the samples investigated. The 0.01–0.1% Ce-doped samples also showed thermally-stimulated luminescence (TSL) with a glow peak of around 90°C after X-ray irradiation. The TSL response of 0.01–0.05% Ce-doped samples increased monotonically with X-ray dose over a dose range of 10^{-1}–10^{4} mGy.

(GFMAT-P041-2019) Scintillation properties of tellurium oxide glasses doped with europium

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We investigated photoluminescence (PL) and scintillation properties of tellurium oxide glasses doped with different concentrations of Eu (0.1, 0.5, 1.0 and 5.0 mol.%). The Eu-doped samples were fabricated by the conventional melt-quenching method. Emissions due to the 4f-4f transitions of Eu^{3+} were observed in PL and scintillation. Among the samples investigated, 5% Eu-doped sample showed the highest intensity in PL and scintillation. In addition, the decay time constants of the Eu-doped samples in PL and scintillation were a few milliseconds, which were typical decay time constant of the 4f-4f transitions of Eu^{3+}.

(GFMAT-P042-2019) Scintillation properties of Yb^{2+}-doped strontium halide crystals

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Ce^{3+} and Eu^{2+} have been extensively studied and applied as activators in various scintillators because of their fast and efficient parity-allowed 5d–4f emissions. In contrast, the potentially suitable divalent lanthanide Yb^{2+} has rarely been used, although it has been previously studied as a luminescence center for other applications. Yb^{2+} exhibits a ground-state closed-shell $4f^{14}$ configuration, and is therefore stabilized in the solid state. Moreover, its ground state is similar to Eu^{2+}, which has a half-filled $4f^{7}$ configuration. In this study, we examine the photoluminescence and scintillation properties of Yb^{2+}-doped SrX_2 (X = Cl, Br, I). The light yields of $SrCl_2$:Yb^{2+} and $SrBr_2$:Yb^{2+} were determined to be 54,000 and 62,000 photons/MeV, respectively, in comparison with the reference sample NaI:Tl^{+} (40,000 photons/MeV)

(GFMAT-P043-2019) Nucleation Mechanism from Fluoride Segregation in New Transparent Oxyfluoride Nanocrystallized Glasses

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Rare-earth (RE) -doped oxyfluoride glasses and glass-ceramics have been received much attention because of their transparency, formability, and low phonon energy. In this work, new oxyfluoride glasses with (33.3-x/3)BaF_2–xZnO–(66.7-x)B_2O_3 (x=0-50, in mol%) and Er_2O_3-doped compositions were prepared, and luminescence, crystallization, and glass structure were investigated. Radial distribution functions of glasses which were evaluated using synchrotron X-ray diffraction at a beamline of BL-04B2 in SPring-8, Japan. The short-range order, i.e., B–(O,F) and Ba–(O,F), showed almost same distance, on the other hand, the distance between Ba–Ba decreased with addition of ZnO despite of the decrease the concentration of Ba ions in ZnO added samples. In order to investigate the glass structure in detail, molecular dynamic simulation was carried out, and then fluoride segregation was observed in the obtained model with the composition of x=40. In this study, we propose that such segregations of fluoride acts as nucleation sites.

(GFMAT-P044-2019) Synthesis and Luminescence of Layered Organic-Inorganic Perovskite Nanocrystals in Glass

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As organic-inorganic crystals (OI) have unique characteristics not found in conventional inorganic crystals, they have emerged as new candidate materials for lighting and scintillator applications. Confined excitons in quantum structures are attractive phenomena that provide fast decay time and high light yield. Layered OI of $(RNH_3)_2PbX_4$ (R: hydrocarbon group, X: halogen) have multiple quantum well structures with alternating organic-inorganic layers. However, there are problems such as cost and size restriction to use as a bulk. In this research, we attempted to grow organic-inorganic perovskite nanocrystals with layered structure in porous glass pores and to obtain bulk rapidly. We focused on (C6H5C2H4NH3) 2PbBr4 (hereinafter Phe), which shows excellent scintillation characteristics. Phe was solved in DMF, and then porous glass were placed in a flask. After the DMF evaporated, organic-inorganic perovskite in glass (OIiG) was obtained. The OIiG was translucent. From the XRD pattern of the obtained composite, it was confirmed that the precipitated crystalline phase was Phe. The peak position was consistent with the single crystal, and no shift was observed. Spherical nanoparticles with a particle size of 3-4 nm was observed in TEM. The PL spectra were measured, and sharp peak was appeared at 416 nm for OIiG and 408 nm for the single crystal was observe.

(GFMAT-P045-2019) Scintillation and X-ray Storage Luminescence of Sn-doped Zinc Sodium Phosphate Glasses

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Many studies for scintillators and X-ray storage phosphors have been performed for the past decades. These two types of phosphors are mostly single crystals or crystalline powders. Glass materials have advantages of their high transparency, productivity and chemical stability, but there are not so many studies on glass materials for radiation measurements due to their low luminescent efficiencies. In such a situation, the H. Masai's group have recently shown that Sn-doped zinc phosphate glasses exhibit high photoluminescence quantum yields exceeding 90%. Therefore, we are studying scintillation and X-ray storage luminescence properties of Sn-doped phosphate glasses. In this study, Sn-doped zinc sodium phosphate glasses were prepared by a conventional melt quenching method, and their properties were evaluated.

(GFMAT-P046-2019) Radioluminescence Properties of Sn-doped Gallium Oxide Single Crystals

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Inorganic scintillators play an important role to detect ionizing radiation in various fields such as medical imaging, security inspection, and well-logging. While many types of insulator-based scintillators are practically used, relatively few types of semiconductor-based scintillators are used. Among the semiconductor scintillators, ZnS:Ag is well known over several decades and used for charged particle detection. Because the single crystal of ZnS:Ag is difficult to obtain, the crystalline powder is used. Due to its opacity, the detection efficiencies of powders are lower than those of single crystals. Recently, our group reported scintillation properties of a transparent Ga_2O_3 single crystal as the novel semiconductor scintillator, and it showed a high light yield (15,000 ± 1,500 ph/MeV). In this study, we focused on Sn-doped Ga_2O_3 single crystals. The Sn ions can be doped in Ga_2O_3, and can affect its energy band structure. We have grown single crystals of Sn-doped Ga_2O_3 by the floating zone method and investigated scintillation properties of them.

(GFMAT-P047-2019) Scintillation properties of $RE_2Hf_2O_7$ single crystals

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Scintillators convert incident ionizing radiation into thousands of ultraviolet-visible photons, and they have been used in different fields of radiation measurement including medical imaging, security and so on. Among scintillators, heavy element-based materials with high effective atomic number are advantageous in high energy radiation detection. Up to now, $Bi_4Ge_3O_{12}$ scintillator, which were developed in 1973, has been mainly used. In order to develop a scintillator which is a substitute for $Bi_4Ge_3O_{12}$, we focus on hafnium-based oxide as a new heavy element material. Since hafnium-based oxide has a quite high melting point of 2400 °C, it is difficult to grow a single crystal; therefore, only a few studies on hafnium-based oxide polycrystalline powder or ceramic have been reported. In this study, $RE_2Hf_2O_7$ and (M=La, Gd, Lu) single crystals were synthesized using Floating Zone furnace with Xenon lamp, which is suitable for crystal growth showing high melting point materials. We evaluate the photoluminescence and scintillation characteristics of these crystals for the first time.

(GFMAT-P048-2019) Evaluation of $Sm:SrCl_2$ single crystal scintillators

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Scintillators convert incident ionizing radiation into thousands of ultraviolet-visible photons, and they have been used in different fields of radiation measurement including medical imaging, security and so on. Among scintillators, heavy element-based materials with high effective atomic number are advantageous in high energy radiation detection. Owing to a strong broad emission due the 5d-4f transitions, Ce^{3+} and Pr^{3+} have been introduced to practical scintillator materials such as Ce:GAGG and Pr:LuAG. Although Sm^{2+} also shows 5d-4f emission, there has been only a few reports on Sm^{2+}-doped scintillator. Since Sm^{2+} shows strong emission from red to near-infrared region, Sm^{2+} is suitable for Si-photodetector and it is easy to distinguish from Cherenkov light. So, Sm^{2+} can be useful emission center in the future. In this study, $Sm:SrCl_2$ single crystal were grown by the vertical Bridgman method, and the photoluminescence (PL) and scintillation characteristics were evaluated.

(GFMAT-P049-2019) Piezoelectric thin films on Si for ultrasonic fingerprint recognition systems

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Secure authentication of one's identity is a major challenge in a modern society due to the increasing popularity of mobile devices (such as smart phones) that can not only store the owner's personal information but also allow banking transactions. A biometrics-based authentication system has attracted a great attention owing to its relatively high-security level and convenience. Current fingerprint recognition systems do not meet the required security level: optical sensors are hard to miniaturize and easily deceived, and capacitive detectors often fail to recognize the patterns by contamination. The ultrasound technology with pMUT (piezoelectric micromachined ultrasound transducer) is one of the most promising technologies to realize such a highly-secure biometrics-based authentication system for mobile electronics. The performance of pMUT is directly determined with the electromechanical property of the piezoelectric layer. However, using conventional piezoelectric materials such as AlN, ZnO, and PZT, it is difficult to generate high power ultrasound that can penetrate into the skin to see veins. Therefore, it is highly desirable to integrate single crystalline relaxor-ferroelectrics, so-called giant piezoelectric materials, on Si substrate. In this talk, I will discuss the issues on the epitaxial integration of $Pb(Mg,Nb)O_3$-$Pb(Zr,Ti)O_3$ thin films on Si.

(GFMAT-P050-2019) Active brazing of Al_2O_3 to copper using dual active filler Ag-Cu-Sn-Zr-Ti for electric vehicle

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Active metal brazing (AMB) using Ag-Cu-Ti active braze alloy is the versatile brazing technique adopted for ceramic to metal joining in automobile and consumer electronic industries. The major problem addressed in AMB is the residual stress along the bonding interface. In the present work a series of dual active Ag-Cu-Sn-x Zr-y Ti (x = 0, 0.8 wt% & y = 0 to 4.2 wt%) fillers were sandwiched between the pieces of Al_2O_3 and high purity copper, and brazed in vacuum furnace to a temperature between 800°C to 900°C for 10 min. Along with Ti_3Cu_3O and Ti_3O_2 phase, $ZrTiO_4$ oxide phase was observed at the Al_2O_3/Ag-Cu-Sn-Zr-Ti interface. The shear strength of Al_2O_3/Ag-Cu-Sn-Zr-Ti interface as a function of Zr composition was evaluated. Acknowledgement: This work was supported by the Technology Development Program (S2517123) funded by the Ministry of SME's and Startups, Korea

(GFMAT-P051-2019) Starch-based processing of porous ceramics with hierarchical microstructure and partially sintered matrix

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Starch and starch-related products have become popular processing additives for porous ceramics. For many applications, hierarchical microstructure can be an advantage. In porous bioceramics (bone tissue engineering), large pores are needed for bone cell ingrowth, while small pores are needed for fluid transport (nutrients, growth factors). Similarly, hierarchically porous ceramics with a porous matrix can offer increased thermal insulation while maintaining sufficient mechanical strength. Here we report on recent achievements in the processing and characterization of highly porous mullite and hydroxyapatite ceramics with hierarchical microstructure and partially sintered matrix, prepared via mechanical foaming with wheat flour, starch and partial sintering. The microstructure has been characterized via stereology-based image analysis, X-ray computed microtomography and mercury porosimetry. It is shown that the method is suitable for ceramic foams with three hierachical

levels of porosity (trimodal pore size distribution) and that the largest and intermediate convex pores (foams bubbles and pores from starch granule burnout) can be efficiently controlled by processing parameters (stirring or shaking time, amount and type of starch), while the smallest concave pores (intergranular porosity) are strongly dependent on the firing temperature. Grain growth is discussed as well.

(GFMAT-P052-2019) Biomaterial with bioactive function and biomaterial with antimicrobial function

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Bioactivity is an indispensable element as a biomaterial. On the other hand, it is also a pointed out that the higher the bioactivity, the breed more bacteria. For that reason, a composite material having each function was developed so that bioactivity and antibacterial function can be selectively given with one base material. Zirconia was selected as a base material and composite material was produced using a material that was easily bonded to zirconia. It was confirmed that the produced composite material had good bioactivity and antibacterial activity. In one test piece, both bioactivity and antibacterial property can be imparted. This developed product having these multiple functions is expected as a new biomaterial.

(GFMAT-P053-2019) Porous ceramic grafts made via unit-by-unit additive manufacturing

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Calcium phosphate porous ceramics are utilized as bone grafts for regenerative medicine. Ideally, geometrical features of pores in the bone grafts should be designed for new bone formation as well as liquid transport. However, rules of designing pore geometries are still unclear. This is partly because geometrical features of the pores in conventional porous ceramics are random, then it is hard to find out effective geometrical features from bone repair trial using these porous ceramics. To address theseissues, I have developed an original porous ceramics fabrication, which builds porous ceramics as a unit-assembly. The fabrication, first prepares small ceramic units with describable geometries, for example, f1 mm spherical unit with a f300 mm through hole. Then, assembles the units up to a required figure. The assembly can be fixed by sintering or casing. In the assembly, an inter-unit gaps form network without dead space. The assembly can function as a porous ceramic graft with describable pore shapes, required figure, and robust inter-unit gaps. In this presentation, details of the method will be introduced with some topics relating to hydroxyapatite units and its assembly.

(GFMAT-P054-2019) 3D ultra-porous bone graft bioceramic materials via SLA

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It is widely known that the main requirements for bone tissue engineering materials are biocompatibility, resorbability and osteoconductivity. Nowadays the most promising resorbable materials for bone implantation are calcium phosphate bioceramics (e.g. based on tricalcium phosphate $Ca_3(PO_4)_2$). Osteoconductive properties of materials are mainly determined by the total porosity of the material, pore size and distribution and the scaffold architecture. As well known, the total porosity should not be less than 70%, and the size distribution of pores should be at least bimodal to provide the scaffold permeability and surface roughness. Moreover, to increase the permeability, it is necessary to have an additional directed pore system (with a diameter of at least 500 μm) in the form of straight channels in several directions. Creation of porous materials with complicated architecture is possible only using additive manufacturing techniques including stereolithography (SLA), which is one of the most universal and precise methods. In this work, we propose a new type of 3D-printed osteoconductive materials (scaffolds) for bone implantation, which have ultra-porous (the porosity more than 85%) specific architecture (gyroid and diamond) with a complex (multimodal) system of pores of at least three levels. The work was supported by RSF, grant #18-79-00256. The authors acknowledge partial support from Lomonosov Moscow State University Program of Development.

(GFMAT-P055-2019) Fabrication and investigations of thermoelectric properties of organic thin film devices

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Global warming is one of the biggest concerns for the future of our planet and its inhabitants. In this regard, thermoelectric materials get one of the main topics of research in terms of waste heat recovery directly through the Seebeck effect while being independent on the light existence. Inorganic, rare earth elements are the first choice for thermoelectric applications. In fact, these materials (e.g., Te, Bi, Pb) are rare, toxic and manufactured using expensive processes, thus hampering the widespread use of thermoelectrics. In sharp contrast, organic materials are cheap, carbon-based and solution-processable while having flexibility. In this work, IIDDT-C3-isoindigo and bithiophene based conjugated polymer with alkyl chains on both sides- (p-type semiconductor) is used to fabricate oriented thin film devices with Langmuir-Schaefer method and chemically doped with FTS to improve their hole mobility which is directly related to the thermoelectric figure of merit (zT). Prepared devices present promising progress in terms of the role of morphological anisotropy and the effect of doping with the focus in high electrical conductivity (σ) combined with a large Seebeck coefficient (S). The outcomes of this research include an understanding of thermal/electric transfer within the active layer of devices to be used in highly small, flexible, low-cost electronics.

(GFMAT-P056-2019) Thermoelectric performance of p-type BiSbTe based materials coated by ZnO via an atomic layer deposition

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Thermoelectric materials, which allow the direct conversion of heat to electric energy and vice versa, have drawn attentions for applications of sustainable energy through scavenging from waste heat. Creation of structural defects including nanoinclusion, interfaces, and grain boundaries through nanostructuring has achieved higher thermoelectric efficiencies mainly due to the significant reduction in the thermal conductivity. However, it is still challenging to optimize the nanostructure via conventional fabrication techniques. The thermal instability of nanostructures remains issues in the reproducibility of the fabrication and long-term stability during the operation. Here, we present a versatile strategy to create numerous interfaces in a thermoelectric material via an atomic layer deposition (ALD) technique. A very thin ZnO layer was conformally formed by ALD over the BiSbTe powders, and numerous heterogeneous interfaces were generated from formation of BiSbTe -ZnO core-shell structures even after high-temperature sintering. The exquisite control in the ALD cycles provides a high thermoelectric performance of zT = 1.50 ± 0.15 (at 329 – 360 K). The high thermoelectric performance through the grain boundary engineering via the ALD is also proved in the

thermoelectric module fabricated with the p-type BST/ZnO legs and commercial zone-melt n-type legs.

(GFMAT-P057-2019) Development of RuO_2 thin film prepared by photo-assisted metal-organic deposition

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Considering the recent global interest in reducing energy consumption, SiC power electronics technology is now ready to enable the step to the next plateau for efficiency standards. In most case, SiC power modules are designed to work at operating temperatures around 250 ºC. Therefore, a comical available electronic components such as resistor, cannot use for the SiC modules because the electrode and resistor materials is deterioration in the temperature. In addition, we found that the trimming part is not good for the heat cycling properties (-40-250ºC). To overcome this problem, we developed RuO_2 thin film on polyimide substrate for resistor by using a photo reaction of hybrid solution (PRHS) process. In this presentation, we will explain the PRHS process for the thin film resistor, and its electrical properties.

(GFMAT-P058-2019) Flexible Transparent Conducting Thin Film Prepared by Photo Chemical Solution Process For Flexible Electronics

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An ITO films on a glass or a plastics substrates were prepared by the photo reaction of nano-particles (PRNP). We have successfully obtained an ITO thin film by the photo reaction of the nano-particles (PRNP) using an excimer lamp and laser at room temperature without vacuum. Using the combined two-step irradiation and one-step irradiation process, the electrical resistivity, carrier concentration, Hall mobility and transmittance at 550 nm of the ITO film were $5.94\times10^{-4}\Omega$cm, 1.05×10^{21} cm^{-3} to and 9.99 cm^{-2} V^{-1} s^{-1} and 81%, respectively. Based on the TEM results, improvement of the resistivity of the film is found to be due to the formation of the large grain size by the laser irradiation. Also, N_h of the ITO films prepared by PRNP process is found to be much higher than that of the film by simple thermal process of nano-particles. ITO film on PET was prepared by PRNP process. The Sheet resistance of the film on PET is 85Ω/sq. Transmittance of the film at 550nm is 83%. In addition, to improve the sheet resistance, photo reaction of hybrid solution process was developed. By using the hybrid solution process, the Sheet resistance of the film on PET is 54Ω/sq. It was found that PRHS is effective for the preparation of the ITO film on plastics substrate at low temperature.

(GFMAT-P059-2019) Measurement of mechanical properties of SiC coating using microcantilever beam specimens

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SiC coating is widely used for surface modification. Although mechanical proeprties, such bending strength and fracture toughness, of the ceramic coating are important to understand its performance, they have not be measured directly, yet. In this study, mechanical properties of SiC coating prepared by laser CVD were measured using microcantilever beam specimens. The SiC coarting was amorphous composed of Si, C and small amout of O. The microcantilever beam specimens were fabricated by the FIB technique on the ion-polished surface of the SiC coating. The specimen size was 0.5 μm × 0.9 μm × 4 μm. Loading the tip of the specimens was carried out using nano-indenter. Young's modulus calculated from the initial stage of the stress-strain curve was 471±99.5 GPa, which was in good agreement with those of single crystal SiC. The microcantilever beam specimens plastically deformed and then fractured, even at room temperature as is the case of single crystal SiC. The fracture toughness of the amorphous SiC coating was 2.5 $MPam^{1/2}$, and it was within the value of single crystal SiC measured using bulk sample. The bending strength of the coating was 32.8±2.78 GPa. Although the measured value was lower than the ideal strength of single crystal SiC, it also seems to be ideal strength because ab-initio calculation showed that amorphization and C/Si ratio decrease the ideal strength.

(GFMAT-P060-2019) Numerical Modeling of the Lamellar Domain Damage in MMC

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The metal/ceramic composite obtained by infiltration of the high porous ceramic preform by aluminum alloy are investigated. The ceramic perform is produced by freeze-casting process and has lamella microstructure due to ice crystals growth during the freezing of ceramic slurry. The resulting microstructure of the composite is very complex and only application of the numerical modeling allows prediction of its thermo-mechanical behavior. In our previous studies the material model based on the 2D images of the real microstructure was developed. By development of this model was supposed that the microstructure of the composite is not changing in the freeze-casting direction. In this paper, a single-domain sample of metal-ceramic composite with lamellar microstructure is modelled theoretically using a combination of analytical and computational means. Stress field in the ceramic layer containing multiple transverse cracks (with and without widening) is determined using a modified 2-D shear lag approach and a finite element method. The non-linear shear stress distribution in the shear layer was estimated using a finite element method and implemented in analytical solution. Degradation of stiffness properties of the sample due to multiple transverse cracking is predicted using the equivalent constraint model.

(GFMAT-P061-2019) Synthesis of Stable β-$PdH_{0.43}$ nanocrystals with Controllable Structure and Their Catalytic Activity towards Formic Acid Oxidation

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To understand the structure-property relationship of nanocatalysts is very meaningful and it may facilitate to design a promising catalyst with high performance. Pd cube, octahedra (Oct) and rhombic dodecahedra (RD) are enclosed by the {100}, {111} and {110} facets, respectively. In this paper, we developed a simple solvothermal method to convert these three different Pd nanocrystals into stable $PdH_{0.43}$ nanocrystals. The $PdH_{0.43}$ nanocrystals still maintains its original morphology despite the existence of lattice expansion. During the process of conversion, we have found that the all three Pd nanocrystals can form a stable structure of $PdH_{0.43}$, but cubes show the fastest speed in forming of $PdH_{0.43}$ nanocrystals and the best thermal stability, followed by Oct and RD. Finally, we use formic acid electrooxidation as a probe reaction to better understand the structure-performance relationship, the order of highest oxidation current density is $PdH_{0.43}$ cube > $PdH_{0.43}$ Oct > $PdH_{0.43}$ RD, and the oxidation potential after forming $PdH_{0.43}$ ware all reduced a lot, $PdH_{0.43}$ cube reduced the most, which is close to 190 mV negative comparing to that of Pd Cube.

(GFMAT-P062-2019) Impact of electric field and grain size on thermal conductivity of spin thermal conductivity film

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Recently, considerable waste heat is emitted from electric devices, but almost all of the heat has not been reused. In order to reuse that heat energy, it is required to develop a new device to actively control heat flow like light and electricity. Therefore, the purpose of this study is to develop a novel thermal management material and we have focused on spin thermal conductivity materials, e.g., $La_5Ca_9Cu_{24}O_{41}$ (LCCO), which has anisotropic, high thermal conductivity derived from spin arrangement. Thus, we have attempted to control thermal conductivity of the LCCO by applying electric field for controlling spin arrangement. In this report, we have prepared multilayers comprising LCCO, SiO_2, and sandwich electrodes and have investigated impacts of applied electric fields on the thermal conductivity of LCCO by using frequency-domain thermoreflectance method. In addition, for the achievement of the high thermal conductivity, we investigated the effects of the grain size on the thermal conductivity.

(GFMAT-P063-2019) Compositional engineering to novel bismuth-based organic-inorganic hybrid halide perovskites

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Lightning fast growth in the power conversion efficiency of methylammonium lead iodide ($CH_3NH_3PbI_3$) based perovskite solar cells (PSC) over the past 4-5 years, has attracted a lot of attention in the field of photovoltaic research. However, poor stability in the warm and humid conditions has been a prime concern, which is needed to be addressed before it can be used for commercial purpose. In the current investigation, we have synthesized novel bismuth-based photo absorbers with perovskite (ABI_3) crystal structure to counter the poor moisture resistance. Thin films of these samples have been made by spin coating technique followed by annealing at optimized temperature. The XRD and XPS studies have confirmed hexagonal crystal symmetry and elemental homogeneity of these materials respectively. Micrometer range large crystals with hexagonal morphology have been found in the FE-SEM as well as fluorescence image microscopy study. UV-Vis spectra have shown high absorption in the visible spectrum with an optical band gap at around 1.8 eV. Time correlated single photon counting spectroscopy (TCSPC) measurement has exhibited charge carrier recombination time on the order of a picosecond. Furthermore, no such noticeable change recorded in the XRD patterns as well as UV-Vis spectra even after two weeks' time period, demonstrating superior stability.

(GFMAT-P064-2019) Nb and La doped $SrTiO_3$ oxides and nanocomposites for high temperature thermoelectric power generation

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Concept of recycling the waste heat by thermoelectric power generator is an efficient way of producing electricity, since 60% of the energy used in all kinds of combustion engines and industries is wasted in the form of heat. In recent years, oxide thermoelectric material arises to be promising candidate over chalcogenides and intermetallics due to its high temperature stability and low processing cost. $SrTiO_3$ stands out of the queue because of its large Seebeck coefficient, though it suffers from high thermal conductivity. Here we report significant increase in thermoelectric device figure of merit (ZT) in $SrTiO_3$ based oxides, compositionally modified by Nb and La doping. Further we have shown that enhancement of ZT values can be obtained by forming their nanocomposites by inducing phonon scattering at the interfaces, resulting low thermal conductivity without affecting its electrical conductivity. Bulk ceramics of all the compositions have been synthesized by spark plasma sintering. Phase purity and microstructure analysis have been carried out by XRD, XPS, SEM. Further various thermoelectric parameters such as electrical conductivity, thermal conductivity and Seebeck coefficient have been measured in the temperature range from 300 K to 1100 K in order to estimate ZT values for these perovskites and nanocomposites.

(GFMAT-P065-2019) Enhanced thermoelectric performance of 20% Nb-doped $SrTiO_3$: Effect of Spark Plasma Sintering

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Recently, Nb-doped $SrTiO_3$ has drawn intense attention as high temperature n-type thermoelectric material because of its lucrative features for device application. In this work, 20% Nb-doped $SrTiO_3$ (STN20) was synthesized by Spark Plasma Sintering (SPS) route to investigate the effect of SPS on the thermoelectric performance of the fabricated material. XRD and FESEM studies confirmed the presence of single phase in the solid solution with highly dense and non-porous microstructure which is achieved by the employment of SPS method. Temperature dependent electrical conductivity measurement showed semiconductor to metal (S-M) transition at ~ 430K. The highest value of thermoelectric power factor of 439.88 $\mu W/m\text{-}K^2$ was achieved at around 760K. STN20 ceramics exhibited glass like behavior resulting in low thermal conductivity. Furthermore, dimensionless thermoelectric figure-of-merit (ZT) was also calculated for this material to estimate its potential for device application, where we obtained the maximum value of ZT = 0.14 at ~ 1050K. However, further investigations need be pursued to enhance the thermoelectric properties by preparing composites of STN20 with such materials which possess high electrical conductivity but low thermal conductivity.

(GFMAT-P066-2019) Tensile Creep Behaviors of Lap-Spliced Carbon Fiber-Textile Reinforced Cementitious Mortar Composites

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In the present study, tensile creep behaviors of lap-spliced carbon fiber-textile aluminum cement-based mortar (TRM) composites were experimentally investigated through tensile creep test. Two different treatment details at lap-spliced area of textile were used as test parameters including: carbon fiber textile impregnated by epoxy, and carbon fiber textile coated with aluminum oxide powder after epoxy impregnation. Also, the effect of lap-spliced length was also investigated. The lap-spliced lengths were 170 and 200 mm. All test specimens were subjected to a sustained load corresponding to 30% of tensile strength of mortar according to time progress. The environmental conditions including temperature and humidity were kept at 20±2ºC and 65±10%, respectively. From the test, the tensile creep behaviors were measured and investigated. The results showed that the tensile creep of the TRM composites could be significantly influenced by the lap-spliced length as well as the surface treatment. In addition, the sustained load effect on the tensile creep of the materials was understood.

(GFMAT-P067-2019) Characterizations of Sr_2CeO_4 ceramics for scintillator applications

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Inorganic scintillators, which convert high energy ionizing radiation to thousands of photons, have been playing a major role in many fields of radiation detection, including medicine and security. In this study, we have synthesized a series of Sr_2CeO_4 ceramics sintered at different temperatures by solid-state reaction. Then, we investigated the scintillation and photoluminescence properties such as X-ray induced scintillation spectra, scintillation decay curves, pulse height spectra under ^{137}Cs γ-ray irradiation, PL excitation/emission spectra and PL decay curves. In X-ray induced scintillation spectra of Sr_2CeO_4 ceramic samples, an emission peak at 510 nm was observed in all the samples. Similar emission peak was also reported by the earlier work, in which the origin of this mission was ascribed to ligand-to-metal CT. Then, we measured pulse height spectra of all the Sr_2CeO_4 samples measured under ^{137}Cs γ-ray irradiation. The absolute light yields were derived as relative values to that of conventional $Y_3Al_5O_{12}$:Ce crystal scintillator. The derived absolute light yield was 3,200 ph/MeV.

(GFMAT-P068-2019) Defects as luminescence centres in long persistent phosphor of α-$Na_xZn_{3-0.5x}(PO_4)_2$

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A light bluish green long-lasting phosphorescent (LLP) material α-$Na_xZn_{3-0.5x}(PO_4)_2$ was prepared using a conventional solid-state sintering technique. The samples were characterized by X-ray diffraction (XRD), photoluminescence (PL), and thermoluminescence (TL) techniques. The emission band locates at around 460 nm, being fitted to be two peaks at 455 nm and 501 nm with Gaussian fitting, respectively. TL curves show that the dopant of Na^+ ions and heating reducing atmosphere largely enhance the concentration of defects. The possible luminescence mechanism is proposed.

(GFMAT-P069-2019) Luminescence mechanism and enhancement of a red long persistent phosphor γ-$Zn_3(PO_4)_2$: Mn^{2+} by doping Mg^{2+}

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A red long persistent phosphor of γ-$Zn_3(PO_4)_2$: Mn^{2+}, Mg^{2+} was prepared through homogeneous coprecipitation and conventional solid-state sintering methods. The crystalline structure and property of samples were confirmed by utilizing X-ray diffraction, the photoluminescence spectra, and the thermoluminescence (TL) spectra. The X-ray diffraction phases indicate that the dopant of Mg^{2+} is responsible for the phase conversion of $Zn_3(PO_4)_2$: Mn^{2+} from α to γ as well as the improvement of the crystallinity of phosphors. Photoluminescence emission spectrum of the red γ-$Zn_3(PO_4)_2$: Mn^{2+}, Mg^{2+} phosphor shows a strong prominent peak at 620 nm due to the transition of $^4T_{1g}$-$^6A_{1g}$ of Mn^{2+} ion. The luminescence properties of γ-$Zn_3(PO_4)_2$: Mn^{2+} can be effectively enhanced by the dopant of Mg^{2+}. The long-lasting phosphorescence was observed for about 2 h with naked eyes in the dark after the irradiation light sources have been removed. The TL curves are employed for the discussion of intrinsic defects. The working mechanism of the persistent luminescence was proposed.

(GFMAT-P070-2019) Optical and scintillation properties of Ce-doped $Ca_3Sc_2Si_3O_{12}$ single crystal

T. Kato*[1]; N. Kawaguchi[1]; T. Yanagida[1]

1. Nara Institute of Science and Technology, Japan

A scintillation light yield (LY) is greatly correlated with a quantum yield (QY) in photoluminescence (PL), and it is common that a phosphor with a high QY shows a high LY. In this study, we focused on $Ca_3Sc_2Si_3O_{12}$ (CSSG) of which the crystal structure is the same garnet as $Y_3Al_5O_{12}$ and $Gd_3Al_2Ga_3O_{12}$. PL properties of a Ce-doped CSSG were reported, and it emits strong yellowish green light due to 5d-4f transitions of Ce^{3+} ions under excitation light. Therefore, in this study, we synthesized Ce-doped CSSG single crystal using by the floating zone (FZ) method. After the synthesis, we measured optical and scintillation properties. When X-ray was irradiated, the Ce-doped samples showed an intense emission band peaking around 510 nm, and the emission wavelength was close to that of Ce-doped YAG and GAGG. Pulse height spectra were measured under ^{57}Co exposure. Clear photoabsorption peaks were detected in the Ce-doped samples. The absolute light yield was determined as 4,000 ph/MeV.

Wednesday, July 24, 2019

G2: Novel, Green, and Strategic Processing and Manufacturing Technologies

Novel, Green, and Strategic Processing II

Room: Trinity IV
Session Chairs: Kiyoshi Shimamura, National Institute for Materials Science; Yoshitake Masuda, National Institute of AIST

8:30 AM

(GFMAT-101-2019) Novel single crystals for electro-optical applications: Growth and characteristics (Invited)

K. Shimamura*[1]; V. Garcia[1]

1. National Institute for Materials Science (NIMS), Japan

Electro-optical technology progress in a wide range of applications, and still demands the further development. Here, recent activities of our group related with novel single crystals with advantageous characteristics will be reviewed. A new concept of high-brightness white LEDs based on Ce:YAG single crystal phosphor plates (SCPPs), which can overcome the conventional temperature- and photo-degradation problems, is proposed. SCPPs demonstrated excellent thermal stability with no temperature quenching, high values of luminous efficacy and increased quantum efficiency. $Tb_3(Sc_{1-x}Lu_x)_2Al_3O_{12}$ (TSLAG), CeF_3 and PrF_3 single crystals have been designed and grown for high-power laser machinery. They showed a higher visible-UV transparency and a larger Faraday rotation than $Tb_3Ga_5O_{12}$. They are therefore very promising material in particular for new magneto-optical isolator applications in the UV-VIS-NIR wavelength. $K_{1-x}Na_xNbO_3$ (KNN) lead-free single crystals are attracting much attention for various piezoelectric applications due to their relatively high piezoelectric coefficient and high Curie temperature. In this work, KNN single crystals were successfully grown. The properties of grown crystals were systematically studied. Authors would like to thank to Koha Co., Ltd., and Fujikura Ltd., for the collaboration.

9:00 AM

(GFMAT-102-2019) Novel, Green, and Strategic Processing of Ceramic Nanomaterials for Sensors: SnO_2, TiO_2, ZnO (Invited)

Y. Masuda*[1]

1. National Institute of AIST, Japan

Metal oxide nanocrystals have been attracted much attention for functional devices. In this study, sophisticated shapes of SnO_2, TiO_2 or ZnO nanocrystals were developed in aqueous solutions for a molecular sensor, a gas sensor, a hydrophilic coating, an anti-reflective coating, etc. Nucleation and crystal growth were controlled to synthesize characteristic nanostructures. A sensor has been developed for detecting 1-nonanal gas present in the breath of lung cancer patients by combining SnO_2 nanosheets with SnO_2 nanoparticles and noble metal catalysts. A significant change in the electrical resistance of this sensor was observed with increasing 1-nonanal gas concentration; the resistance decreased by a factor of 1.12 within the range of 1 to 10 ppm at 300 °C. High sensitivity is attributed to the accelerated oxidation of 1-nonanal molecules caused by the (101) crystal faces of the SnO_2 nanosheets and should provide a simple and effective approach to the early detection of lung cancer.

9:30 AM

(GFMAT-103-2019) Glass and Ceramic Drilling Using Fiber Lasers (Invited)

S. Jiang*[1]

1. AdValue Photonics Inc, USA

Fiber lasers have attracted intense interest in recent years because of its outstanding performance compared to other types of lasers for industrial application. Recently glass and sapphire laser processing have become necessary because of the need for a variety of applications. In this presentation, we present our latest studies of picosecond and nanosecond high peak power and high repetition rate green fiber lasers at 515nm for glass and sapphire drilling applications.

10:20 AM

(GFMAT-105-2019) Localized plasticity in SiC ceramics induced by laser shock processing

F. Wang[1]; X. Yan[1]; C. Zhang[2]; L. Deng[2]; M. Nastasi[1]; Y. Lu[2]; B. Cui*[1]

1. University of Nebraska-Lincoln, Mechanical and Materials Engineering, USA
2. University of Nebraska-Lincoln, Electrical and Computer Engineering, USA

Laser shock processing (LSP) is a novel surface engineering technique, in which a nanosecond-pulsed laser irradiates the ceramic surface to generate a plasma. The explosive expansion of the plasma generates laser-driven shock waves that can penetrate into the bulk material. Compared to metals, LSP has not been widely applied to ceramic materials, and the fundamental mechanisms of LSP on ceramics are less understood. Transmission electron microscopy characterizations discovered significant dislocation activities near the surface and grain boundaries in LSP-treated SiC ceramics, suggesting that the localized plasticity can be generated during the LSP process at room temperature. As a result, a high compressive residual stress was generated from the surface to a depth of 750 μm, which was revealed by X-ray diffraction analysis. The LSP-induced localized plasticity can improve the mechanical properties of SiC ceramics, such as the bending strength and fracture toughness.

10:40 AM

(GFMAT-106-2019) SiC/VSi2 for different uses

J. Narciso*[1]; A. Ortega[1]; M. R. Caccia[1]

1. Alicante University, Spain

SiC is a material widely used in a large number of applications, ranging from catalysis (embryonic phase) to composite materials. However, one of the unresolved problems is the manufacture of SiC parts at a reasonable cost. With the appearance of reactive infiltration, costs have been significantly reduced. This has led to a small reduction in its mechanical properties. However, the main problem with these systems is that their use can not be higher than 1000 C, due to residual silicon. In our research group we have developed a large number of strategies to solve this problem. They range from the use of silicon alloys, to a strict control of the carbon material used, as well as its porous structure. In the present communication, the results for the Si-V system are shown. A basic study of the process of infiltration and wetting of liquid alloys with carbon substrates is carried out, and their final properties are analyzed

G3: Crystalline Materials for Electrical, Optical and Medical Applications

Optical Materials III

Room: Salon C
Session Chairs: Nerine Cherepy, Lawrence Livermore National Lab; Philippe Goldner, Chimie ParisTech

8:30 AM

(GFMAT-108-2019) Novel waveguide Bragg grating structures produced by femtosecond direct laser writing (Invited)

R. Laberdesque*[1]; Y. Petit[1]; H. Fares[1]; A. Abou-Khalil[2]; S. Danto[1]; I. Manek-Hönninger[2]; T. Cardinal[1]; L. Canioni[2]

1. CNRS, ICMCB, France
2. University of Bordeaux, CELIA, France

Direct Laser Writing (DLW) with ultrafast near-IR lasers in silver-containing phoshapte glasses allows for the formation of sub-micron scale distributions of silver clusters (100 nm for the smallest dimensions), with remarkable optical responses: refractive index modification, strong fluorescence contrast, second- and third-harmonic generation, and even up to surface plasmonic resonance. These properties allow for the 3D implementation of optical functions, such as the creation of non-conventional single-mode waveguides provided by laser inscription of double-track structures made of silver clusters. In this contribution, we show successful femtosecond DLW in an original configuration leading to integrated ridge waveguide Bragg gratings with periods of 300 to 250 nm, for which first-order Bragg resonances are expected in the visible range. A demonstration of proof-of-concept is in progress, which would allow to further design waveguide Fabry-Perot cavities for innovative integrated laser devices.

9:00 AM

(GFMAT-109-2019) Development of Advanced Oxide Thin Films Prepared by Ultraviolet Laser Reaction for Electrical and Optical Applications (Invited)

T. Tsuchiya[1]; T. Nakajima[1]; I. Yamaguchi*[1]; J. Nomoto[1]; Y. Uzawa[1]

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

To construct AI and IOT society more and more in the world, it is necessary to develop a high performances new flexible sensor device. Metal oxides are expected to be key materials which are used for a new device by controlling metal composition, a crystal structure, orientation or multilayer of the film, a carrier, a spin, etc. However, in most case, heat treatment at greater than 500ºC is required for the crystallization of the oxide thin film, it is difficult to prepare oxide thin film on plastic substrates. Thus, it is necessary to develop the low temperature processing for flexible electronics usin oxide materials. For this aim, we have developed the photo-induced chemical solution process such as excimer laser-assisted metal organic deposition (ELAMOD) and photo reaction of nano-particle (PRNP). By using their methods, epitaxial VO_2 film and flexible VO_2 film were prepared at low temperature. By controlling the ingredient crystallinity and oxygen contents of the films, high temperature coefficient of resistance (TCR) of the VO_2 film(=32%/K) was obtained. In addition, flexible

$La_{1-x}Sr_xMnO_3$ film was successfully obtained on Y_2O_3/metal substrate without the oxidation. In this paper, we explain the epitaxial thin film and flexible thin film by ELAMOD and its excellent properties.

9:30 AM

(GFMAT-110-2019) Additive Manufacturing of Transparent Ceramics (Invited)

Z. M. Seeley*[1]; T. Yee[1]; N. Cherepy[1]; S. A. Payne[1]

1. Lawrence Livermore National Laboratory, Materials Science Division, USA

Polycrystalline transparent ceramics offer a few advantages over single crystal or glass optical materials, including mechanical toughness and near-net shape manufacture. A unique opportunity that optical ceramics fabrication provides is the ability to form a tailored composition profile throughout the 3-dimensional bulk of the optic. Unlike most glass and single crystal optics, ceramics are fabricated from a solid green body and densified through a solid-state sintering process. This process allows a green body with tailored composition, such as a doping gradient, to retain its compositional profile through to the final optic. Among others, laser gain media appears to be one application which could significantly benefit from a tailored doping profile, promising to improve laser efficiency, mode control, and wavefront. We have successfully fabricated core-clad Nd:YAG rods with a doping profile and achieved lasing when installed in a commercial laser head. Additionally, Yb:YAG waveguides have been optimized to achieve single mode propagation. Compositionally tailored optics will soon find uses in other applications. This work was performed under the auspices of the U.S. DOE by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-765918

10:20 AM

(GFMAT-111-2019) Unique Advanced Transparent Oxide Ceramics Films (Invited)

T. Yamamoto*[1]; Y. Furubayashi[1]

1. Kochi University of Technology, Research Institute, Japan

Science and industry alike are realizing that transparent-oxide-ceramics films hold many interesting “frontier” properties: electrical, optical and antibacterial properties. We propose a materials design to tailor film properties for wide applications. The key factors are to control carrier concentration in a wide rage together with carrier transport and to manipulate reactive oxygen species at the film surfaces. We have been developing a unique film growth apparatus, reactive plasma deposition with dc arc discharge. It enables us with low-temperature deposition of crystalline oxide films on amorphous glass or flexible polymer substrates. For the fabrication of high efficiency of 24.1% Si-based hetero-junctions solar cells, recently, we have succeed in the co-doping method using Ce and H atoms to achieve In_2O_3-based transparent electrodes exhibiting high Hall mobility of more than 145 cm^2/Vs and low free carrier absorption in the near-infra red wavelength spectral range. The processing temperature is of less than 200 °C. Very recently, we have been developing the state-of-the-art technology to generate and irradiate electronegative oxygen (O^-) ions. The use of O^- technology is an effective way to manipulate a density of oxygen-related defects or generates reactive oxygen species in the vicinity of surface of ZnO conductive films. The applications include glass or polymer substrates with antibacterial oxide transparent materials.

10:50 AM

(GFMAT-112-2019) Fabrication of transparent polycrystalline ceramics by colloidal processing and SPS (Invited)

T. S. Suzuki*[1]

1. National Institute for Materials Science, Ceramics Processing Group, Japan

Transparent polycrystalline ceramics provides flexibility in size and shape design to apply for a wide field. Extremely low porosities are indispensable for high transparency. In general, high temperature needs to eliminate pores, but high temperature enhances large grain growth. Spark plasma sintering (SPS) is effective way for densification in low sintering temperature and grain is prevented from growing. Furthermore, Colloidal processing is a very effective technique for controlling the pore size distribution in green compacts before sintering. The green compacts having small residual pores with a narrow size distribution is expected to enhance the densification at low sintering temperature during SPS. In this presentation, this processing was applied to fabrication of transparent alumina, AlN and AlON. Commercially available alumina and AlN powder was used as the starting materials. Slurries with 30 vol% solid were consolidated by slip casting. The green compacts before sintering were further densified by cold isostatic pressing at 392 MPa for 10 min. Final sintering was carried out using an SPS. The transparency of alumina prepared by colloidal processing was higher than that densified by SPS from the as-received powder. In the case of AlON, after slip casting of the mixture of alumina and AlN, transparent AlON was obtained by reactive sintering during SPS.

11:20 AM

(GFMAT-113-2019) Rapid Sintering of Alumina by Laser Irradiation (Invited)

T. Kimura*[1]

1. Japan Fine Ceramics Center, Japan

Two important techniques for laser sintering of alumina have been developed; (a) a drying/dewaxing technique of slurry layer, and (b) effective laser heating technique. In this study, an alumina slurry containing sub-micron alumina powder was used as a starting material. By controlling temperature distribution in the coated slurry layer using a hot-plate heating, the slurry layer was dried and dewaxed without crack, and densely packed alumina powder layer (green density: 83~86%) was obtained. The dense powder layer was also obtained by spraying the slurry onto the pre-heated substrate. Nd:YAG laser (wavelength:1064 nm) was employed in this study as a heating source, but alumina poorly absorb this laser. We formed a graphite layer on the alumina powder layer as an absorption aid to assist the laser heating of the alumina layer, and 300 micron-thick layer was successfully sintered by 10 seconds irradiation at power density of 250 watt/sq-cm. Furthermore, laser sintering of a bulk alumina body was also investigated, and a transparent alumina consist of an mm-order single crystals (sapphire) was obtained.

G5: Advanced Functional Materials, Devices, and Systems for Environmental Conservation, Pollution Control and Critical Materials

Advanced Functional Materials, Devices, and Systems VII

Room: Trinity III
Session Chairs: Kazuhiko Maeda, Tokyo Institute of Technology; Katsuro Hayashi, Kyushu University

8:50 AM

(GFMAT-114-2019) New opportunities in chemistry from mixed-anion compounds (Invited)

H. Kageyama*[1]

1. Kyoto University, Japan

Mixed anion compounds, which contain several different anions, began to draw attention as game-changing inorganic materials. Since, compared with conventional inorganic compounds such as oxides, mixed-anion compounds may exhibit unique coordination and resultant extended structures, from which fundamentally different chemical and physical property may emerge. My talk aims to describe the current status and scope as well as outline future challenges surrounding mixed-anion (oxide-based) compounds.

In particular, a special focus is given to oxyhydride (oxide-hydride) materials. For example, $BaTiO_{2.6}H_{0.6}$ is found to be a good starting material that allows a hydride-exchange reaction to occur at low temperatures, yielding oxynitride, $BaTiO_{2.6}N_{0.3}$ and $BaTiO_{2.5}H_{0.25}(OH)^{0.25}$. Such reactivity or lability of hydride anion makes the $BaTiO_{2.6}H_{0.6}$ a novel catalyst for ammonia synthesis, which is unprecedented since titanium was long thought as a 'dead' element for this applications. The utmost feature of hydride that differentiate it from other anions is the lack of π-symmetry in the valence shell, which explains a recently found insulator-to-metal transition in $SrVO_2H$ under high pressure. The high-pressure X-ray diffration study on $SrVO_2H$ revealed that the hydride anion is two times as compressible as the oxide anion. The hydride size flexibility is used to drive a novel anion order-disorder transition.

9:20 AM

(GFMAT-115-2019) Design and development of layered mixed anion compounds for future functional materials (Invited)

H. Ogino*[1]

1. National Institute of Advanced Industrial Science and Technology (AIST), Electronics and Photonics Research Institute, Japan

The compounds containing more than one anionic species in a single phase, so-called mixed anion-compounds, have been considered as a new family of functional materials. Layered mixed-anion compounds, composed by stacks of different kind of layers show novel properties such as high temperature superconductivity, transparent conductivity, and high thermoelectric property materials due to their specific crystal structures. Recently we developed a series of layered compounds composed by semiconducting and insulating layers such as $Sr_2ScCuSO_3$. These compounds show sharp exciton emission peaks near the band edge, and the stability of excitons at room temperature because of quantum confinement effect owing to their layered structure. We have also discovered several related compounds. Chemical flexibility of the functional layer offers to tune the band gap of the compounds, and structural difference gives different level of the quantum confinement effect as well as temperature stability of the luminescence.

9:45 AM

(GFMAT-116-2019) Effect of Nitrogen/Fluorine Codoping into Rutile TiO_2 on Its Photocatalytic Activity

A. Miyoshi*[1]; J. J. Vequizo[2]; S. Nishioka[1]; Y. Kato[3]; M. Yamamoto[4]; S. Yamashita[5]; T. Yokoi[1]; S. Nozawa[6]; A. Yamakata[2]; T. Yoshida[3]; K. Kimoto[5]; K. Maeda[1]

1. Tokyo Institute of Technology, Japan
2. Toyota Technological Institute, Japan
3. Osaka City University, Japan
4. Nagoya University, Japan
5. National Institute for Materials Science (NIMS), Japan
6. High Energy Accelerator Research Organization, Japan

Significant efforts have been made to develop photocatalysts that functions under visible light from the viewpoint of solar energy utilization. Nitrogen doping into TiO_2 has been studied intensively as a way to obtain a visible-light-responsive photocatalyst. Nitrogen/fluorine codoping into anatase TiO_2 has been reported to enhance nitrogen incorporation compared to only nitrogen-doped one, resulting in higher visible light absorption and photocatalytic activity. On the other hand, rutile TiO_2 (R-TiO_2), another representative polymorph of TiO_2, is known to possess high photocatalytic ability for O_2 evolution via water oxidation and used with suitable H_2 evolution photocatalyst to achieve overall water splitting by the scheme called Z-scheme. Here, we succeeded in introducing visible light response into R-TiO_2 by N/F codoping for the first time and evaluated its O_2 evolution activity. It was revealed that fluorine codoping not only enhance nitrogen introduction, but also suppresses formation of defect states (and/or oxygen vacancies), which reduces photocatalytic activity. Furthermore, N/F codoped R-TiO_2 was shown to be applicable for O_2 evolution photocatalyst in Z-scheme water splitting in combination with Ru loaded Rh doped $SrTiO_3$ (H_2 evolution photocatalyst), in the presence of $[Co(bpy)_3]^{3+/2+}$ (bpy = 2,2′-bipyridine) as a redox mediator under visible light and simulated sunlight.

Advanced Functional Materials, Devices, and Systems VIII

Room: Trinity III

Session Chairs: Hiroshi Kageyama, Kyoto University; Hiraku Ogino, National Institute of Advanced Industrial Science and Technology (AIST)

10:20 AM

(GFMAT-117-2019) Photocatalytic and Photoelectrochemical Water Splitting and CO_2 Fixation using New Mixed-Anion Compounds (Invited)

K. Maeda*[1]

1. Tokyo Institute of Technology, Japan

Water splitting and CO_2 fixation using semiconductor photocatalyst and photoelectrodes are of importance from the viewpoint of solar-to-fuel energy conversion toward artificial photosynthesis. Mixed-anion compounds that consist of more than two anionic species in a single-phase have attracted attention as visible-light-driven semiconductors, because as compared to oxygen 2p orbital, p orbitals of less electronegative anion can form a valence band that possesses more negative potential. In this talk, recent progress on the development of new mixed-anion photocatalyst and photoelectrodes that are applicable to water splitting and CO_2 fixation will be given. It had been believed that oxyfluorides are unsuitable as visible-light-responsive photocatalysts because of the highest electronegativity of fluorine. Surprisingly, $Pb_2Ti_2O_{5.4}F_{1.2}$ possessed an unprecedented small band gap of ca. 2.4 eV, and functioned as a stable photocatalyst for visible-light water reduction/oxidation and CO_2 reduction when modified with suitable promoters. Density functional theory calculations showed that the unprecedented visible-light-response of $Pb_2Ti_2O_{5.4}F_{1.2}$ arises from strong interaction between Pb-6s and O-2p orbitals, which is caused by a short Pb–O bond in the pyrochlore lattice due to the fluorine substitution.

10:45 AM

(GFMAT-118-2019) Fabrication of ceria-zirconia particles with high specific surface area by microwave-emulsion method (Invited)

M. Inada*[1]; J. Hojo[2]

1. Kyushu University, Center of Advanced Instrumental Analysis, Japan
2. Kyushu University, Faculty of Engineering, Japan

In this study, CeO_2-ZrO_2 spherical particles with high specific surface area were fabricated by microwave-emulsion method. The microemulsion method is one of the effective processes to synthesize spherical oxide particles, in which W/O emulsion consists of oil phase as matrix and water phase as micelle surrounded by emulsifier. When the microwave is applied to microemulsion process, the oil phase does not absorb microwave, and the water phase including reactants is selectively heated under microwave irradiation, leading to stable formation of spherical oxide particles. Spherical CeO_2-ZrO_2 particles formed as cubic crystal phase, in which many small pores were included in the spheres. The solid solution was generated after the heat treatment without morphological change. The oxygen absorption capacity of CeO_2-ZrO_2 is useful as oxidation catalyst. The changes in particle morphology and oxygen storage property with Ce/Zr ratio are discussed on the basis of formation mechanisms.

11:10 AM

(GFMAT-119-2019) Titanium Carbonitride Nanoflakes Converted from MXene by Nitrogen Gas Annealing (Invited)

K. Hayashi*[1]; K. Nishimi[1]; N. Tsuruno[1]; K. Kimoto[3]; G. Hasegawa[1]; M. Inada[2]

1. Kyushu University, Department of Applied Chemistry, Japan
2. Kyushu University, Japan
3. National Institute for Materials Science (NIMS), Japan

Formation of titanium carbinitride $TiC_{1-x}N_x$ nanoflakes from $Ti_3C_2T_x$ MXene as a precursor has been investigated. The titanium carbonitride flakes that inherit the morphology of the MXene are available by simply heating in pure N_2 atmosphere. The conversion process includes the decomposition of surface functional groups on MXene laminates up to ~800 °C and the nitridation to form the titanium carbonitride with rock-salt structure in ~800-1000 °C. During this process, fine carbonitride flakes with thicknesses a few tens nm are formed so as to exfoliate the MXene grains with thicknesses of ~1 μm, leading to the high surface are of ~20 m^2/g. To explain a deep nitridation in the product, we propose that CO desorption derived from oxygen in the surface functional groups markedly affects the degree of the nitridation and relevant x value. The MXene-derived titanium carbonitride is characterized by the nitridation process without ammonia, and the various shapes from flakes, coatings and even to bulks, providing a wide range of applications including electrochemical electrodes with a low-dimensional morphology with high surface area.

11:35 AM

(GFMAT-120-2019) Two-Dimensional MXene and Their Composites: Synthesis and Applications (Invited)

J. Zhu*[1]

1. Shaanxi University of Science and Technology, School of Materials Science and Engineering, China

MXenes, a new family of two-dimensional (2D) early transition metal carbides and carbonitrides, have been receiving a significant research interest by virtue of their excellent electrochemical energy storage properties, high electrical conductivity, and superior mechanical properties. The precursor MAX phases Ti_3AlC_2 and Ti_2AlC, as well as some bimetal composites with high purity have been successfully obtained by hot pressing method. MXenes are successfully prepared by etching Al from precursor MAX in HF. To obtain MXene with few and/or single layer, the etching time is lengthened. Another mature synthesis route to layered MXene is HCl/LiF etching, which is assisted by mild sonication. Also, we focus on the surface modification of MXene and MXene-based composites, with probable synergistic effect in agglomeration prevention, facilitating electronic conductivity, improving electrochemical stability and enhancing pseudocapacitance. Here, we summarize the development and progress of our work in synthesis of various MXene and modifications to MXene-based composites, focusing on their performances and applications as mediator-free biosensors, Li-ion batteries, supercapacitors and photocatalyst materials.

G7: Ceramics Modeling, Genome and Informatics

Prediction of Structure and Performance I

Room: Trinity I
Session Chair: Yanwen Zhang, Oak Ridge National Laboratory

8:30 AM

(GFMAT-121-2019) Effects of Electronic and Nuclear Energy Dissipation on Nanostructure Evolution (Invited)

W. J. Weber*[1]; E. Zarkadoula[2]; Y. Zhang[2]

1. University of Tennessee, Materials Science and Engineering, USA
2. Oak Ridge National Lab, Materials Science and Technology, USA

Ion-solid interactions result in energy loss to electrons and atomic nuclei. Using computational and experimental approaches, we have investigated the separate and combined effects of electronic and nuclear energy loss on the response of ceramics to ion irradiation. The loss of energy to electrons results in significant ionization and formation of hot electrons that create a local thermal spike via electron-phonon coupling. Using molecular dynamics (MD) simulations and the inelastic thermal spike model, the coupled effects of the nuclear and electronic energy loss have been investigated. Amorphous tracks are readily produced with high energy ions in many ceramic oxides above a threshold in electronic energy loss. We have discovered that, in some complex oxides, amorphous tracks can be produced below this threshold due to the spatial coupling of electronic and nuclear energy dissipation processes or to a synergy between the electronic energy dissipation processes and pre-existing defects. These results provide new insights into the complex processes involved in the coupling of electronic and atomic dynamics. Work supported by the U.S. Department of Energy, Basic Energy Science, Materials Science and Engineering Division.

9:00 AM

(GFMAT-122-2019) Hydrogen Storage Materials and Hydrogen Economy (Invited)

R. Ahuja*[1]

1. Uppsala University, Physics and Astronomy, Sweden

The purpose of this talk is to provide an overview of the most recent theoretical studies undertaken by us in the field of hydrogen storage materials research. On selected examples, the application of our computational tool of choice, density functional theory, will be illustrated to show how ab initio calculations can be of use in the effort to reach a better understanding of hydrogen storage materials and to occasionally also guide the search for new promising approaches. A deeper theoretical understanding of the catalytic mechanism involved in kinetic enhancement should be a very valuable guide in the design of new catalysts. Systems to be discussed include complex metal hydrides. Catalysis play an important role in many hydrogen desorption processes. We found (through a combination of experiment and theory) that carbon nanostructures, in particular nanotubes and fullerenes, can be used as catalyzing agents for hydrogen uptake and release in complex metal hydrides (such as sodium alanate, $NaAlH_4$) and provide a model which could explain the mechanism of the catalytic effects.

9:30 AM

(GFMAT-123-2019) Thermochromic VO_2 for smart windows: A view from first principles calculations (Invited)

Y. Cui*[1]; B. Liu[1]; Y. Gao[1]

1. Shanghai University, China

VO2 presents a metal-insulator transition, which can automatically adjust the near-infrared light transmittance with temperature changes and can be applied to smart windows. The thermochromic property of VO2 is due to its unique electronic structure and atomic structure,

namely the strong correlation of V-3d electrons and the arrangement of V-V bonds. This report summarizes the first principles calculations progresses on VO2 from the perspectives of bulk materials, intrinsic point defects and surface/interface. We first calculated the influence of 29 kinds of transition metal element doping on the atomic structure of VO2 bulk material. It was found that the volume expansion of VO2 lattice and the decrease of lattice constant β angle after doping were closely related to the decrease of phase transition temperature. Secondly, it was found In the VO2 intrinsic point defect, oxygen vacancies can increase the electron concentration of VO2, lower the phase transition temperature, dimerize the R-phase VV chain, narrow the M-phase band gap, and enhance the near-infrared absorption. Thirdly, studies on the VO2/nobel metal interface found that the charge is transferred from the noble metal to the surface of VO2, and the surface dipole moment is enhanced. By adjusting the ratio of V to the noble metal atom, the surface work function of VO2 can be changed to regulate the phase transition temperature.

Prediction of Structure and Performance II

Room: Trinity I
Session Chair: William Weber, University of Tennessee

10:20 AM

(GFMAT-124-2019) Ab Initio Molecular Dynamics Studies of Low-Energy Recoil Events in Functional Oxides

Y. Zhang*[1]; B. A. Petersen[2]; B. Liu[3]; H. Xiao[4]; W. J. Weber[2]

1. Oak Ridge National Laboratory, USA
2. University of Tennessee, Materials Science and Engineering, USA
3. Shanghai University, China
4. University of Electronic Science and Technology of China, China

Ab initio molecular dynamics is carried out to investigate low-energy recoil events in oxides with rock salt (MgO), fluorite (CeO_2, ZrO_2, and ThO_2), perovskite ($SrTiO_3$, $LiNbO_3$ and $LiTaO_3$) and pyrochlore ($Gd_2Zr_2O_7$ and $Gd_2Ti_2O_7$) structures, which are important materials for advanced electro-optical, photonic and nuclear energy applications. Studies on threshold displacement energy (E_d) along specific crystallographic directions, the role of charge transfer on the dynamics of the recoil process and defect production, and the final defect configurations and charge redistribution have revealed that the recoil events involve partial-charge transfer assisted processes. The effective charge for the primary recoil atom varies significantly to overcome the energy barrier for defect formation. Charge redistribution leads to new defect configurations and charge states due to the delocalization of electrons on neighboring atoms. The non-equilibrium charge effect can impact functionality. This work was supported by the Office of Basic Energy Sciences, U.S. Department of Energy.

11:00 AM

(GFMAT-125-2019) Diurnal variation detector concept for dark matter particles (Invited)

K. Nordlund*[1]

1. University of Helsinki, Finland

Many astrophysical observations indicate that standard model particles compose only 5% of the matter in the universe. Understanding the nature of dark matter and dark energy, the remaining 85%, is of fundamental importance to cosmology, astrophysics, and high energy particle physics. There are a number of attempts for direct detection of dark matter particles via an elastic interaction with detector nuclei. To date, the detectors developed could detect dark matter particles with masses > 10 GeV/c^2. In our recent work, we showed that potential dark matter particles in the mass range down to 200 MeV/c^2 could be detected by new kinds of single-electron resolution single crystal semiconductor detectors. Moreover, since the threshold displacement energy depends on crystal direction, while the dark matter particles do not follow Earths rotation around its axis, the response of a single crystal detector should vary with the time of day. In this work, we used classical and time-dependent density functional theory molecular dynamics to calculate the response of the semiconductor detectors to dark matter recoils as a function of crystal direction, and using an analytical model translated this into a dependence of the signal on the time of the day. The diurnal variation could be a major benefit for distinguishing a dark matter particle signal from that of conventional particle physics standard model particles.

G8: Advanced Batteries and Supercapacitors for Energy Storage Applications

K-ion Battery

Room: Salon D
Session Chair: Seung-Taek Myung, Sejong University

8:30 AM

(GFMAT-127-2019) On the way to K-ion batteries: Negative electrodes based on p-group elements (Invited)

V. Gabaudan[1]; J. Touja[1]; R. Berthelot[1]; L. Monconduit[1]; L. Stievano*[1]

1. ICGM, University of Montpellier, CNRS, France

In the last years, many efforts have been devoted to the development of novel battery systems based on Earth abundant elements such as sodium, magnesium and more recently potassium. The latter provides several benefits in terms of ionic conductivity in organic electrolytes, energy density (originating from its low standard potential), abundance and cost. However, several drawbacks of K-ion batteries (KIB), such as the high atomic mass and Shannon ionic radius of K^+ compared to Li^+ and Na^+, cast some doubts about their possible competitiveness compared to Li-ion and Na-ion systems. As a proof of concept, the detailed electrochemical mechanism of a series of electrode materials based on C, Sn and Sb in KIB, uncovered via complementary operando and ex situ analyses, will be presented. The influence of the different mechanisms on their cycling performance will be highlighted, showing advantages and drawbacks of the different materials. In particular, it will be shown how the activation of tin is possible only in synergy with a second metal, which modifies its reaction path through the formation of different and more reversible intermediates.

9:00 AM

(GFMAT-128-2019) Advancing Materials Research For Rechargeable Potassium Ion Batteries (Invited)

T. Masese*[1]; K. Yoshii[1]; M. Kato[1]; K. Kubota[1]; H. Senoh[1]

1. National Institute of Advanced Industrial Science and Technology (AIST), Energy and Environment, Japan

There is a crucial need to meet the world's enormous energy demands in a sustainable manner with low environmental impact. Lithium-ion (Li-ion) battery technology, as an alternative to cater to these energy demands, faces a projected scarcity of its terrestrial mineral reserves. To address the increasing demand for large-scale rechargeable batteries, particularly for volume/weight-less-dependent applications such as the electric grid system, the development of new low-cost alternatives to Li-ion batteries but with comparable performance is a worldwide imperative. Rechargeable potassium-ion (K-ion) batteries (KIBs) are gaining traction as not only low-cost battery alternatives, but also as high voltage energy storage systems. However, the development of KIBs is particularly plagued by the lack of suitable structural materials for reversible insertion of the large K-ions. Exploration of the broad minerals and compounds database relating to potassium-based materials aided with computational chemistry has led us to pinpoint new materials that are capable of reversible K-ion insertion at high voltages. Materials exploration through computational chemistry may serve as a milestone for materials research in the development of K-ion battery, which is still at its infancy stage. We will highlight our recent progresses in developing materials for rechargeable K-ion batteries.

9:30 AM

(GFMAT-129-2019) High Voltage Sodium and Potasium-ion Batteries by Concentrated Aqueous Electrolytes (Invited)

S. Okada*[1]; K. Nakamoto[1]; R. Sakamoto[2]; M. Ito[1]

1. Kyushu University, Institute for Materials Chemistry and Engineering, Japan
2. Kyushu University, Interdisciplinary Graduate School of Engineering Sciences, Japan

As high-cost performance large-scale rechargeable battery, inexpensive aqueous Na-ion battery using the amount of resources rich sodium and high safety aqueous electrolyte is attractive. However, the cathode and anode active materials not only have low solubility and high chemical stability against water, but also each redox potential must be located within the narrow electrochemical potential window of water. Recently, 3 V-class Li-ion batteries with concentrated aqueous electrolytes have been reported. On the other hand, although aqueous Na-ion battery is more attractive as high-cost performance large-scale rechargeable battery, there are few reports about high voltage aqueous Na-ion battery more than 2 V. In order to realize the higher cost performance rechargeable battery, we focus on the Na-ion battery with high concentrated $NaClO_4$ aqueous electrolyte with inexpensive prussian blue based organic cathode and anode. In this study, 2 V discharge will be demonstrated in aqueous Na-ion battery with $Na_2Mn[Fe(CN)_6]$ cathode and $KMn[Cr(CN)_6]$ anode. Among Prussian blue analogs, $KMn[Cr(CN)_6]$ is used as anode for the first time. Because it is cheaper and has lower potential than the conventional anode active materials such as NASICON-type $NaTi_2(PO_4)_3$ in aqueous Na-ion batteries. It can be used as anode for aqueous K-ion battery, also.

Organic Materials for Battery

Room: Salon D

Session Chair: Shigeto Okada, Kyushu University

10:20 AM

(GFMAT-130-2019) Further Insights into the Interfacial Chemistry of Organic Electrode Materials for Li-ion batteries (Invited)

A. Naylor[2]; D. Brandell[2]; S. Renault*[1]

1. Institut des Matériaux Jean Rouxel (IMN), France
2. Department of Chemistry – Ångström Laboratory, Sweden

The formation of a solid electrolyte interphase (SEI) is well-known and characterized for inorganic LiB materials. However, it has been scarcely investigated for organic electrode materials (OEMs). It is speculated that the formation of a less stable SEI layer for OEMs and its evolution during battery cycling could be at the origin of several issues for these batteries such as decreasing capacity or loss of material during cycling. One of the main reasons for these scarce studies is due to the difficulty to distinguish the OEMs contribution from the decomposition materials coming from either OEMs or electrolyte, which are all composed of the same elements (C, H, O, Li). We recently investigated the electrochemical behaviour of dilithium 2-aminoterephthalate, a nitrogen-containing OEM. Further investigations on this material, its complexation ability and a battery design/electrode formulation free of any other sources of nitrogen permitted us to perform a thorough X-ray photoelectron spectroscopy (XPS) study. Using N 1s core level peaks as a marker, we were able to discriminate the signals of different elements depending of their origin. The results will be presented with the aim to improve the comprehension of some electrochemical features of OEMs.

10:50 AM

(GFMAT-131-2019) Organic cathode materials for Mg batteries (Invited)

J. Bitenc*[1]; K. Pirnat[1]; T. Bančič[1]; A. Vizintin[1]; A. Randon Vitanova[2]; R. Dominko[1]

1. National Institute of Chemistry, Department of Materials Chemistry, Slovenia
2. Honda R&D Europe GmbH, Germany

Li-ion batteries are currently a dominant battery technology on the battery market, but given the increasing demands for cheaper and more energy dense materials, different alternatives are actively explored (Li-S, Li-O_2, Na-ion, metal-organic batteries). Among those organic materials are especially interesting given the fact that they can be used with different counter ions (Li, Na, Mg, K) and enable application of various metal anodes. Our group is heavily involved in the development of Mg-organic batteries, where we have applied different compounds from the class of anthraquinones, benzoquinones and polyimides. Organic cathodes have shown long-term cycling stability in Mg electrolytes, which opens a route for future developments of Mg-organic batteries. Currently, a major challenge is elucidation of electrochemical mechanism of organic cathodes. To address this question we have developed a simple, operando ATR-IR characterization method, which allows us measurement of cathode IR spectra during battery operation through Si wafer of the modified pouch cells. ATR-IR spectra of the organic cathode confirmed that electrochemical mechanism is the same as in the case of Li batteries. However, a practical realization of Mg-organic batteries will depend on the volumetric density, cathode areal loadings and amount of electrolyte needed for practical cells, which are still the questions that need to be answered.

11:20 AM

(GFMAT-132-2019) Water processable binders for aqueous rechargeable lithium ion battery

E. Tomassi[1]; J. Profili[2]; S. Rousselot[1]; L. Hadidi*[1]; L. Stafford[2]; M. Dollé[1]

1. Université de Montreal, Chemistry, Canada
2. Université de Montréal, Physics, Canada

Rechargeable lithium-ion battery (LIB) with organic electrolyte has found many applications. Its high energy density and long cycle life make it the best option compared to other secondary batteries. However, the fabrication cost, safety concerns, environmental impact on disposal and recyclability remain the main drawbacks for large-scale applications. Hence, interest in aqueous electrolyte rechargeable LIB (ARLB) has grown, particularly for safe and cost-effective large-scale devices. To reduce the adverse environmental/human impact of LIB production, the electrode preparation process needs to be revisited. Replacing common binders (e.g. fluorine-containing polymers; polyvinylidene difluoride (PVDF)) and noxious organic solvents (e.g. N-methyl-2-pyrrolidone [NMP]) by non-toxic and aqueous processable binders is a must. Carboxymethyl cellulose (CMC) has gained considerable attention due to its natural abundance, water processability and lower cost. Nevertheless, using water soluble binder to prepare electrodes for aqueous batteries is unattainable because of its solubility in aqueous electrolytes. We successfully addressed this issue by developing a green water-based strategy to prepare electrode employing CMC for ARLB. Physico-chemical properties and electrochemical performance of the electrodes were investigated. The results are quite promising and comparable to those of organic processed electrodes.

11:40 AM

(GFMAT-133-2019) Active Material/Carbon Nanotube Electrodes: A Versatile Architecture For High Energy Density Lithium Batteries

S. Rousselot*[1]; P. Antitomaso[1]; L. Savignac[2]; S. Genereux[1]; L. W. Taylor[3]; T. Bibienne[1]; M. Pasquali[3]; S. B. Schougaard[2]; M. Dollé[1]

1. Université de Montréal, Chemistry, Canada
2. Université du Québec à Montreal, Chemistry, Canada
3. Rice University, Dept of Chemical and Biomelecular Engineering and Dept of Chemistry, USA

Conventional composite electrodes consisting of a mixture of active material, carbon black and polymeric binder spread on a metallic current collector could impede the development of high energy density batteries as a large part of its composition only act as dead weight. Binder-free, self-standing and flexible electrode only made of active material (AM) and single wall carbon nanotubes (SWNT) have recently been investigated. AM/SWNT electrodes with up to 95 wt.% of active material could be prepared and used in various battery configurations. In this presentation, this electrode architecture is first described and used in liquid electrolyte lithium batteries where the high electronic conductivity promoted by the CNT network allows the stable cycling of coated and even uncoated $LiFePO_4$ as AM. Still, some performance loss evidenced that the SWNT network did not ideally incorporate some AM particles. The architecture was then optimized to reach very high energy density by polymerisation of the 3,4-ethylene-dioxythiophene (EDOT) directly within the electrode. With help of SWNT and PEDOT, a conductive network between the particles is targeted from the macroscopic to microscopic scale.

G14: Advanced CMCs: Processing, Evaluation, and Applications

Advanced CMCs: Processing Evaluation, and Applications

Room: Trinity II
Session Chairs: Emmanuel Boakye, UES Inc.;
Marina Ruggles-Wrenn, Air Force Institute of Technology

8:30 AM

(GFMAT-134-2019) Development of non-oxide ceramic matrix composites for application in advanced gas turbine (Invited)

H. Klemm*[1]; C. Steinborn[1]; K. Schönfeld[1]; A. Michaelis[2]

1. FhG IKTS Dresden, Germany
2. Fraunhofer IKTS, Germany

Ceramic matrix composites (CMC) offer a high potential for applications as structural parts in advanced gas turbines. During recent years, significant progress in material development of oxide and non-oxide CMC has been achieved, however, there are still considerable deficits especially in the long-term behavior of the materials at elevated temperatures. Besides the development of CMC with superior corrosion resistance in hot gas atmospheres, the mechanical behavior of CMC with high damage tolerance crack was found to be one of the most important challenges for these applications in aero engines. In the present study SiC/SiCN composites were fabricated by a precursor infiltration and pyrolysis process (PIP). Several matrix systems with and without fiber coating were used in order to achieve a flaw tolerant behavior. The composites were analyzed regarding their mechanical properties. Special emphasis was placed on the crack formation and propagation behavior in correlation to the microstructural features of the composites. Finally some idea about the design of flaw tolerant CMC will be provided.

9:00 AM

(GFMAT-135-2019) Thermal History Mapping Technology for Turbine Engine Diagnostics (Invited)

K. N. Lee*[1]; C. Pilgrim[2]

1. NASA Glenn Research Center, Materials & Structures, USA
2. Sensor Coating Systems, United Kingdom

The infusion of ceramic matrix composites (CMCs) in next generation gas turbines represents daunting challenges as the failure of protective coating, known as Environmental Barrier Coating (EBC), means little remnant life of CMC components. Consequently reliable lifing is critical to the success of CMC components. Accurate thermal mapping of EBC in rig and engine test is of paramount importance because temperature is the most critical variable for EBC life. Current temperature measurement technologies include thermocouples, pyrometers, IR cameras, and thermal paints. Thermocouples require a passage to access the components and pyrometers and IR cameras require line-of-sight. Thermal paints are based on color-sensitive pigments that visually indicate the temperature that a component experienced. Thermal paints do not require line-of-sight, however, they have a low resolution and a limited temperature capability (~1400°C). Thermal history coating is based on oxide ceramic which luminesces when excited with a light source. The luminescence changes when the material's structure changes triggered by heat impact. The maximum temperature to which the material was exposed can be determined from the luminescence change. This paper describes the principles of this new technique and demonstrates its capabilities for EBCs exposed to excess of 1500°C.

9:30 AM

(GFMAT-136-2019) Static Fatigue of Hi-Nicalon™-S Fiber at Elevated Temperature in Air, Steam and Silicic-Acid-Saturated Steam

S. Robertson[1]; M. Ruggles-Wrenn*[1]; R. Hay[2]; T. Shillig[1]; R. Mitchell[1]; B. Kroeger[1]; L. Gumucio[1]

1. Air Force Institute of Technology, Aeronautics & Astronautics, USA
2. Air Force Research Laboratory, USA

A facility for testing SiC fiber tows in static fatigue at elevated temperatures in air, in steam and in steam saturated with silicic acid was developed. Static fatigue of Hi-Nicalon™-S fibers was investigated at 800-1100° C at stresses ranging from 115 to 1250 MPa in air, in steam, and in steam saturated with silicic acid. The presence of steam reduced fiber lifetimes under static fatigue. Fiber lifetimes were much shorter in unsaturated steam than in $Si(OH)_4$(g)-saturated steam. The Monkman-Grant (MG) relationship was applied to the stress-rupture experimental results. The test environment had little influence on the MG parameters. The MG relationship was demonstrated to successfully predict creep lifetimes in air, steam and steam saturated with silicic acid.

9:50 AM

(GFMAT-137-2019) Manufacturing and testing of a novel hybrid nozzle assembly based on liquid silicon infiltration

L. F. Klopsch*[1]

1. DLR - German Aerospace Center, Ceramic Composites and Structures, Germany

The increasing exploration and use of space and the associated costs require not only the optimization of the launch masses of rockets but also an increase in the specific performance of the engine. Fiber-reinforced ceramic matrix composite structures, which can be used in rocket nozzles, connect these two components. By reducing the mass of the engine, an increase in performance and payload capacity can be achieved. The development of a novel hybrid design of a nozzle assembly including the qualification test on the European Sounding Rocket Range (ESRANGE) will be presented. The production is based on the wet winding technology as well as the liquid

silicon infiltration (LSI) process. Thus the advantages of the high mass specific characteristic values and the high temperature resistance can be used in areas of extreme application, whereas areas of lower temperature are ablatively cooled by a CFRP outer shell.

10:30 AM

(GFMAT-138-2019) Critical role of ZrO_2 on Densification, Microstructure Development and High Temperature Erosion Behaviour of Spark Plasma Sintered NbB_2 (Invited)

T. Maity*[1]; N. Gopinath[3]; K. Biswas[1]; B. Basu[2]

1. Indian Institute of Technology Kanpur, Materials Science and Engineering, India
2. Indian Institute of Science, Materials Research Centre, India
3. Indian Institute of Science, Aerospace Engineering, India

The present study for the first time demonstrates the role of ZrO_2 on densification, microstructure and high temperature erosion behaviour of NbB_2 SPSed at 1750°C for 2 min. The adopted processing approach enables to obtain fully dense (99.6% ρ_{th}) NbB_2-ZrO_2 composite and also helps in obtaining better mechanical properties as well as outstanding high temperature erosion resistance properties. The sintered microstructure is characterized by HRTEM/HAADF analysis, which confirms the uniform dispersion of intragranular t-ZrO_2/o-ZrO_2 particles and random distribution of dislocations and asymmetric twins within the NbB_2 and ZrO_2 grains. Detailed investigations of the specimen erosion tested at 800°C using HRTEM reveal the accumulation of large number of dislocations along with fragmented NbB_2 grains on eroded surfaces indicating the activation of dislocation plasticity during high temperature erosion. The sintered NbB_2-ZrO_2, revealed a combination of properties such as hardness ~22 GPa, flexural strength ~598 GPa, together with moderate short and long crack toughness ~5.2 MPa $m^{1/2}$ and 3.9 MPa $m^{1/2}$ respectively. XRD based residual stresses analysis exhibits simultaneous decrease in tensile residual stress of NbB_2 and an increase in the compressive residual stress of ZrO_2, which aid in improving the erosion resistance at high temperature.

11:00 AM

(GFMAT-139-2019) Manufacture and thermomechanical characterisation of wet filament wound C/C-SiC composites

M. Frieß*[1]

1. DLR - German Aerospace Center, Institute of Structures and Design, Germany

Ceramic matrix composites based on wet filament winding and LSI-processing are attractive candidates (C/C-SiC) for many applications in aerospace. Therefore, commercial C-fibres and a water-based phenolic resin were used for wet filament winding on a mandrel and subsequent curing in an autoclave, followed by pyrolysis to a C-matrix and liquid silicon infiltration (LSI) to form a C-SiC-matrix. By applying wet filament winding the mechanical properties can be tailor-designed according to the chosen fibre orientation since C/C-SiC is a fibre dominant and damage tolerant CMC material. Wet filament winding was performed on a mandrel with winding angles of +/-15°, +/-30° and +/-45°, +/-60° and +/-75° were made possible by cutting samples in perpendicular direction. Tubes in wet state were cut in axial direction, flattened and cured on a flat plate without applying additional pressure, such as warm pressing, in order to obtain similar curing conditions to tubes. Mechanical and thermomechanical characterisation of flat specimen of C/C-SiC composites was performed by using an Indutherm universal testing machine using inductive heating of samples and a laser extensometer for measuring of displacement under inert conditions. Testing of tensile specimens was performed at room temperature as well as high temperatures up to 1600°C. In addition, microstructural characterization was performed by SEM.

11:20 AM

(GFMAT-140-2019) Rare earth disilicate fiber coatings for SiC/SiC CMCs

E. E. Boakye*[1]; P. Mogilevsky[1]; T. A. Parthasarathy[1]; T. Key[1]; M. Cinibulk[2]; R. Hay[2]; S. Opeka[1]

1. UES Inc., Materials Science, USA
2. Materials and Manufacturing Directorate AFRL, USA

Rare-earth disilicates ($RE_2Si_2O_7$) are potential oxidation-resistant alternatives to carbon or BN fiber coatings for SiC/SiC CMCs. Our prior work experimentally demonstrated that rare earth disilicates may work as a weak interface in fiber-reinforced SiC/SiC CMCs. However, the effect of oxidation, especially in water vapor, on their functionality as a weak interface has not yet been tested. In this work, SiC/SiC mincomposites with $Y_2Si_2O_7$ interface were exposed to steam at 1000ºC/10h and tensile tested. Minicomposites with BN interfaces were used as control. The effect of steam on the functionality of the two interface coatings was studied and will be reported.

Thursday, July 25, 2019

G2: Novel, Green, and Strategic Processing and Manufacturing Technologies

Novel, Green, and Strategic Processing III

Room: Trinity IV
Session Chairs: Paul Kim, Rutgers University; Baoqiang Li, Institute for Advanced Ceramics, Harbin Institute of Technology

8:30 AM

(GFMAT-141-2019) Carbonate Ceramics for the Reduction of Global Carbon Footprint (Invited)

D. Kopp*[1]; R. Riman[1]

1. Rutgers, The State University of New Jersey, Materials Science & Engineering, USA

Converting captured carbon dioxide (CO_2) into valuable products such as fuels, chemicals, plastics, and building materials is necessary for effective carbon emissions management. Large polluting industries, like the cement industry, must be targeted when developing solutions for rising carbon emissions. This presentation details the innovative steps being taken by researchers at Rutgers University to reduce the embodied energy and carbon footprint of cement production. These steps include (1) changing the cement chemistry from hydratable (Ca_2SiO_4 and Ca_3SiO_5) to carbonatable phases ($CaSiO_3$), and (2) developing a low-temperature synthesis process for said phases. Specifically, this presentation will describe how Hydrothermal Vapor Synthesis (HVS) can reduce the embodied energy of cement production up to 50% by synthesizing $CaSiO_3$ at temperatures as low as 350ºC, and how Low Temperature Solidification (LTS) can use CO_2 to cure the cement, thereby sequestering 300 kg CO_2 per tonne of cement.

9:00 AM

(GFMAT-142-2019) Microwave carbonization for chitosan derived porous carbon and carbon dots for supercapacitor and bioimaging (Invited)

B. Li*[1]; G. Liu[1]; Y. Chen[1]; D. Jia[1]; Y. Zhou[1]

1. Institute for Advanced Ceramics, Harbin Institute of Technology, China

Rapid and high efficient synthesis of functional carbon derived from sustained biomass is crucial problem for scalable synthesis, energy storage and biomedical application. However, synthesis process of biomass derived porous carbon or carbon dots still has the challenges, such as long carbonization time for furnace pyrolysis

and low synthetic yield of biomass derived carbon dots. To rapid synthesize biomass derived porous carbon, we developed microwave carbonization technology to convert zinc chloride($ZnCl_2$) impregnated biomass (including chitosan and carrot) into porous carbon with 4-10 min. The specific surface area and mesopore ratio were as high as 1899 m^2 g^{-1} and of 70%. Rapid microwave carbonization represents a high efficiency route of conversion of biomass into porous carbon for high-performance supercapacitors. To improve the synthetic yield of carbon dots, we proposed the concept of precursor containing carbon-carbon double bonds to boost the synthetic yield and demonstrate record breaking synthetic yield (85.9%) of carbon dots. Carbon dots served as probes for live cell multicolor imaging and exhibit an outstanding protective effect against oxidative stress via inhibiting exogenous and endogenous reactive oxidative species generation in zebrafish.

9:30 AM

(GFMAT-143-2019) Cold Sintering processing of perovskite halides for solar cell applications (Invited)

M. Kumar[1]; P. Bharti[1]; P. A. Jha[1]; P. K. Jha[1]; P. Singh*[1]

1. Indian Institute of Technology (BHU), Department of Physics, India

Current research is focussed on the cost-effective synthesis and stability of perovskite halides, which are high-efficient light absorbing solar cell materials. In this work, a few perovskite halides were synthesized by simple but unique cold sintering method. The structural features of the samples synthesized through cold sintering were found to be in accordance with their thin film counterparts. A comparative of the band gap (on the basis of synthesis technique) suggests the samples synthesised by cold sintering were at par with other synthesis techniques. The synthesized samples are found to be thermally stable as estimated from thermodynamical parameters ΔG and ΔS. The surface and bulk phenomenon were studied using SEM, AFM, impedance and XPS studies. Moreover, stability of the samples was also examined in Sun-light exposure, the I-V curves are recorded in the interval of the 30 minutes over the duration of 3 h in the continuous exposure of AM 1.5G Sun-light. With the time, no significant degradation was observed for $CsPbBr_3$ as evident from I-V plots of the samples. In addition, a negligible change in crystal structure and band gap of the samples was observed after 100 days of synthesis showing the stability of samples in the ambient condition.

10:20 AM

(GFMAT-144-2019) Biogenic metallic nanoparticles: A nanometric trojan horse approach

D. Medina Cruz*[1]; T. J. Webster[1]

1. Northeastern University, Chemical Engineering, USA

Antimicrobial resistance to antibiotics (AMR) and cancer and two of the main concerns that the healthcare system should face nowadays. Current drugs and antibiotic treatments are becoming ineffective or have plenty of drawbacks. Therefore, new alternatives are needed. Traditional synthesis of nanomaterials is subjected to several disadvantages, such as the production of toxic-by-products and harsh conditions. Green nanotechnology is presented as a suitable answer, allowing the generation of nanostructures in a cost-effective and environmentally-friendly approach. Pathogenic bacteria and human cells -both cancer and healthy ones- were used for the synthesis of metallic nanoparticles. Bacteria and cells are cultured in the presence of metallic salts under standard conditions until the generation of nanoparticles, that is followed using microscopy and spectrophotometric techniques. Nanoparticles were used as antimicrobial and anticancer agents using colony counting unit assays and MTS assays, respectively, as well as characterized. Pathogenic bacteria are used for the synthesis of bacteriogenic metallic selenium nanoparticles. These agents were employed as suitable agents with antimicrobial activity against the same bacteria that synthesized them, showing low cytotoxicity for human dermal fibroblasts (HDF) cells. The synthesis of metallic nanomaterials using cancer and healthy cells -HDF and HFOB- is reported. Pure metal nanoparticles –palladium or platinum- and bimetallic structures –such as gold-platinum- are readily synthesized using the cells, and after purification, they are used as anticancer agents. Microbiological agents are successfully used as a synthetic machine for the generation of metallic nanoparticles of different compositions with biomedical properties. Therefore, they are presented as a suitable approach for the synthesis of nanomaterials in a green fashion, overcoming the limitations of traditional nanotechnology.

10:40 AM

(GFMAT-145-2019) Study on Processing of Novel Spinel Transparent Ceramics by Aqueous Gel-casting Technique

H. Wang*[1]

1. Wuhan University of Technology, China

Spinel transparent ceramics with disorder solid solution structure have already been regarded as important candidates for sapphire, due to their outstanding optical and mechanical properties. In order to meet the increasing requirement in various application fields, components with large size and complicated shape are highly demanded. In this work, some novel spinel transparent ceramics have been prepared through aqueous gel-casting shaping technique. The effects of pH value, dispersant, ball-milling time and solid loading on the viscosity of slurries were investigated. The influences of monomer concentration, MAM/MBAM ratio and solid volume fraction on the bending strength and relative density of green bodies were studied. Finally, slurries with high solid loading (>50vol%) and low viscosity (<500mPa•s) were prepared through all above optimized parameters. After casting and calcining, the obtained samples were densified by pressureless sintering and further hot isostatic pressing. The sintered transparent ceramics showed high in-line optical transmittance. The microstructure of green bodies and sintered samples were investigated.

11:00 AM

(GFMAT-146-2019) Ceramic Matrix Nanocomposites Fabricated using Cold Sintering Assisted Synthesis Route

A. Dwivedi*[1]

1. Indian Institute of Technology (BHU), Ceramic Engineering, India

In the present project, recently invented “Cold Sintering Process” (CSP) was used to design ceramic matrix nano-composites of $NaNabO_3$ Nanowire with up to 20wt% of PVDF as filler. The main intention behind choosing CSP method was to prepare ceramic matrix composite with polymer as a filler. Ceramic matrix allows better sample density, temperature stability and increased dielectric properties. With CSP, ceramic and polymer can be cofired at temperature less than 200^0C. Generally, nanoparticles of ceramic materials are used as an initial powder to expedite the process of sintering. For this reason, nano wires of $NaNbO_3$ were used. Sintering is followed by annealing at 300^0C to prevent incongruent melting of grain boundary and increase the crystallinity in the sample. Furthermore, the formation of ceramic matrix in the composite was verified and distribution of polymers in the ceramic matrix was examined by micro-computed tomographic (micro-CT) analysis. DSC-TGA analysis confirmed that these composites are stable up to 350 ^{0}C. Theoretical breakdown strength and energy density werecalculated and found to be as high as 1345 kV/cm and 6.1 J/cm^3 respectively at room temperature. Discharge efficiency of composite materials were calculated using PE loops and found to be 34% for NW/PVDF composites which was increased to 64% on annealing.

Novel, Green, and Strategic Processing IV

Room: Trinity IV
Session Chairs: Reginaldo Muccillo, IPEN; Koji Morita, National Institute for Materials Science (NIMS)

1:30 PM

(GFMAT-147-2019) Electric field-assisted sintering of ceramic materials for sustainable energy production devices (Invited)

R. Muccillo*[1]

1. IPEN, Brazil

Ceramics for energy production in a sustainable development scenario may be produced by recently proposed cost-effective experimental techniques. Examples: oxygen ion (yttria-stabilized zirconia) and proton (rare earth-doped barium cerate and barium zirconate) conducting solid electrolytes for application in solid oxide fuel cells for clean energy supply, mixed oxygen ion-carbon dioxide (samaria-doped ceria/alkaline earth carbonates composites) conductors for carbon dioxide sequestration from the atmosphere for clean environment, thermoelectrics (calcium cobaltite) for devices for energy production in isolated environments. Extensive research work is being pursued on electric field-assisted sintering of these ceramics, looking for optimized procedures for the ceramics industry. Sintering of those compounds by applying an electric field at temperatures and times lower that those used in conventional sintering have been successfully carried out. Dilatometry under electric fields produced specimens analyzed by scanning electron microscopy, scanning probe microscopy, and impedance spectroscopy analyses. The achieved final density, thickness shrinkage, electrical behavior and microstructure of those ceramic compounds, as well as prospects for scaling up the available lab procedures will be shown.

2:00 PM

(GFMAT-148-2019) Nanocrystalline scandia-stabilized zirconia with improved properties after consolidation by high pressure electric field-assisted sintering (Invited)

E. N. Muccillo*[1]; R. L. Grosso[1]; R. Castro[2]

1. Energy and Nuclear Research Institute, Brazil
2. University of California, Davis, Material Science & Engineering, USA

Scandia-stabilized zirconia, ScSZ, is a ceramic oxide-ion conductor with high ionic conductivity at relatively low temperatures (about 500°C). Consolidation of this ceramic material usually requires high temperatures (≥ 1500°C) to achieve high densification, due to its low sinterability. Moreover, ScSZ exhibits a complex phase diagram, including an ordered rhombohedral phase with low ionic conductivity, for doping up to 10 mol% scandia. Phase transition from the high symmetry cubic phase to the ordered rhombohedral phase is prone to occur in microcrystalline ScSZ ceramics. In this work, fully dense nanostructured ScSZ ceramics were obtained by high-pressure electric field-assisted sintering. Nanocrystalline ceramic powders with varying scandium contents were synthesized by a chemical route, followed by consolidation at relatively low temperatures, 700 and 800°C. Structure and microstructure characteristics along with hardness were evaluated in the nanostructured ScSZ ceramics. The grain size dependent cubic phase stabilization was evidenced by Raman spectroscopy. Nanostructured ScSZ with mean grain sizes varying from 8 to 17 nm were obtained according to specific sintering protocols. High degree of translucence and increase of hardness up to ~15 nm mean grain size were observed in dense specimens of ScSZ.

2:30 PM

(GFMAT-149-2019) Fabrication of transparent zinc sulfide by spark-plasma-sintering (SPS) (Invited)

K. Morita*[1]; B. Kim[1]; T. S. Suzuki[1]

1. National Institute for Materials Science (NIMS), Japan

Infrared (IR) transparent materials are important components for IR sensing and light emitting technologies. In particular, since zinc sulfide (ZnS) can exhibit excellent optical transmission at a wide wavelength range from visible to IR. However, since the mechanical properties of ZnS are low, high strength IR transparent ZnS is required. In this study, spark-plasma-sintering (SPS) technique was applied to attain fine-grained and dense materials. Reducing the processing time and temperature using the SPS technique can suppress the grain coarsening, and hence, must be a promising method to achieve high strength transparent ZnS. The ZnS plate SPed at 800ºC exhibits good optical transmission, in which the text is visible through the plate placed directly on the text. This optical transmission can be attained by the fine-grained and dense microstructure. Although several residual pores smaller than 100 nm are observed at multiple grain junctions, the sintered ZnS maintains a fine grain size of about 1 mm. Since the residual pores act as main light scattering sources, those would lower the optical transmission of visible light less than 40%. The fine-grained and highly dense microstructure of the ZnS plate enables a IR transmission higher than 70%. This suggests that the SPS processing is effective to fabricate transparent ceramics at wide wavelength range.

3:20 PM

(GFMAT-150-2019) Spark Plasma Sintering of Mesporous Powders (Invited)

L. Wang*[1]; M. Wang[1]; W. Jiang[1]

1. Donghua University, China

It is well known that nanometer-sized powders with high surface energy could be densified at low temperature. However, obstacles still remain: the troubles in producing amounts of nanometer-sized powders, the strong tendency for nanoparticles to form agglomerates, the difficulties in manufacturing homogeneous compact and the unwanted grain growth in sintering. Therefore it is necessary to find candidates which can meet the demand of high surface energy in solid-state sintering. Recently, we found that the mesporous powders could be consolidated at very low temperature. The reason is that the mesoporous material is a material containing pores, which has extremely high specific surface area. With cooperative function of temperature and pressure during SPS sintering, the mesoporous materials become unstable and these pores will collapse to form pieces following by formation of new surfaces. Thus, the sinterability enhancement occurring in powders with porous structure is amazing, which is expected to be applicable in preparation of dense materials.

3:50 PM

(GFMAT-151-2019) The fabrication of ultrastrong 3Y-TZP and ATZ ceramics by an oscillatory pressure sintering process

Z. Xie*[1]

1. School of Materials Science and Engineering, Tsinghua University, China

The actual strength of ceramics is much lower than their theoretical value due to considerable flaws appearing during powder consolidation. A straightforward approach to improve their fracture strength is to minimize the quantity and size of flaws within ceramics. Here, we report a sintering strategy to consolidate ultrastrong ceramics by introducing oscillatory pressure. We have fabricated a fully dense 3Y-TZP, ATZ ceramics and with a three-point bending strength of up to 1.81 GPa, 2.1 GPa, respectively (approximately twice the strength of that produced by commonly adopted pressureless sintering under similar sintering schedule)— which are the strongest zirconia and ATZ ceramics yet achieved. Strengthening of the material is based on adopting a dynamic oscillatory pressure during sintering to remove various flaws (including agglomerated-pores and micro-pores), strengthen grain boundaries (mainly owing to the formation of a high number density of coherent grain boundaries structure). We believe that this sintering process can be applied to manufacture other ceramics with extremely high strength for structural applications.

4:10 PM

(GFMAT-152-2019) Mechanical Properties of Multi-Material of Carbon-Fiber-Reinforced Plastic/Aluminum Alloy

Y. Sugimoto[1]; D. Shimamoto*[1]; Y. Hotta[1]; T. Ohji[1]

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

Carbon fibers, which are categorized as inorganic materials, are used for reinforcement of plastics (so called, carbon-fiber-reinforced-plastics or CFRP), generating outstanding performance including super lightness and good mechanical properties. Thus, their application to transportation equipment is expected to bring large conservation of energy and great reduction of CO2 emission. When applying CFRP into automobiles, however, their high cost, which is mostly due to expensive carbon fibers and low productivity of the composites, is a great obstacle. Therefore, using multi-materials comprising CFRP and other conventional light materials such as aluminum alloy will be one of the reasonable solutions. In this case, it is very important to control joining properties between CFRP and aluminum alloy. In this study, we studied the strength and deformation properties of multi-material of CFRP/aluminum alloy, focusing particularly on delamination behavior of the joining interface.

4:30 PM

(GFMAT-153-2019) High-throughput Combustion Synthesis of Solid State Ceramic Powders at Electric Field Assisted Ultra-high Temperature

S. Shuang*[1]; H. Li[1]; G. He[1]; Y. Li[1]; J. Li[1]

1. Technical Institute of Physics and Chemistry, CAS, China

High-throughput experiment is the key technology of “material genetic engineering (MGE)”, which provides material database for high-throughput calculation and data mining. It is also significant on improving development speed of new materials and reducing research cost. The aim of this work is to exploit high-throughput preparation and characterization techniques for novel infrared ceramic powders. Firstly, high-throughput dosing equipment for solid ceramic powders was designed and developed to realize multi-channel “dosing-mixing-compacting” of micro-nano ceramic powders. Here three kinds of material systems was carried out by the equipment, including: 1) oxide infrared ceramic system ($NiAl_{2-x}Cr_xO_4$); 2) non-oxide infrared ceramic system (Zr-Ti-C-B system); 3) exothermic reaction system (Al/CuO, Al/MoO_3). Then electric field was applied to induce ultra-high temperature combustion synthesis of multi-channel powders. Here the combustion synthesis process of Zr-Ti-C-B system and their relationship of composition, structure and infrared performance were systematically studied. And the infrared emissivity above 0.8 were obtained through high-throughput preparation and screening. This technology not only shows advantage of rapid screening, but also help to realize energy-saving application in thermal engineering.

4:50 PM

(GFMAT-154-2019) Effect of NiO Content on the Microwave Sintering and Electrical Properties of NiO-YSZ Composite and Ni-YSZ cermet anode for SOFC

K. L. Singh[1]; A. P. Singh*[2]; P. Sharma[1]

1. DAV Institute of Engineering and Technology, Applied Sciences, India
2. IKG Punjab Technical University, Research & Development, India

Effect of microwave sintering on the electrical properties of NiO-YSZ composites has been investigated. Precursor of the composites mNiO-(1-m) 10YSZ with (m=0.2,0.3,0.4,0.5 and 0.6) have been prepared by mixed oxide method and are sintered by both microwave and conventional heating. These composites are then reduced to yield Ni-YSZ and the electrical properties of NiO-YSZ composites and Ni-YSZ cermets have been evaluated using complex impedance analysis. The study of variations in the bulk electrical conductivity of these samples suggests that there are two types of conduction mechanisms working in these composites, one due to YSZ phase and other due to NiO phase. Further, the value of activation energies for both set of the samples have been calculated in the temperature range of 400^0C to 700^0C and are found to be in the range of 0.97eV to 1.21eV. It has been observed that the activation energy of NiO-YSZ conventionally sintered product is higher than corresponding microwave sintered products. The variation in the bulk electrical conductivity with temperature for the reduced Ni-YSZ sample with composition having m=0.5 has been examined. It is found that the conventionally sintered sample of 0.5Ni-YSZ shows no regular pattern whereas the bulk conductivity of microwave sintered samples of same composition decreases with increase in the temperature.

5:10 PM

(GFMAT-155-2019) Comparison of Microwave Processing and Conventional Processing of Sr doped Hydroxyapatite Biomaterial

A. P. Singh*[1]; R. Chdha[2]; C. Sharma[2]; K. L. Singh[3]

1. IKG Punjab Technical University, Research & Development, India
2. IKG Punjab Technical University, Chemical Sciences, India
3. DAV Institute of Engineering Technology, Applied Sciences, India

Among the various cations that are substituted to tailor-made the properties of calcium hydroxyapatite, Sr is most significant due to its effect on bone formation. In the present study the precursor of Sr doped hydroxyapatite, $Ca_{9.5}Sr_{0.5}(PO_4)_6(OH)_2$ has been prepared by mixed oxide method and calcined at 900°C in an electric furnace. The calcined powder was sintered by a conventional method and microwave processing at three different temperatures of 1000°C, 1100°C and 1200°C. The influence of different sintering temperatures and processing techniques has been explored on the structural and morphological properties of the sintered samples. The changes in lattice parameters show that Sr is incorporated into hydroxyapatite lattice. In the calcined powder and sintered samples both HA, $Ca_{9.5}Sr_{0.5}(PO_4)_6(OH)_2$ as well as TCP, $Ca_3(PO_4)$ were present. Microwave sintered samples have a higher amount of hydroxyapatite, less porosity, higher density and greater micro-hardness in comparison to conventionally sintered samples. As compared to conventionally sintered products, microwave sintered products, have more uniform grain size and low percentage of secondary phase.

G3: Crystalline Materials for Electrical, Optical and Medical Applications

Scintillators

Room: Salon C

Session Chairs: Zachary Seeley, Lawrence Livermore National Lab; Takayuki Yanagida, Nara Institute of Science and Technology

8:30 AM

(GFMAT-156-2019) Development of transparent ceramic scintillators (Invited)

T. Yanagida*[1]; N. Kawaguchi[2]

1. Nara Institute of Science and Technology, Japan
2. Nara Institute of Science and Technology, Graduate School of Materials Science, Japan

Scintillators are one of the phosphors, and they are used in ionizing radiation detectors for medical, security, oil-logging, high energy physics and environmental monitoring. Up to now, most of scintillators have been a bulk single crystal due to their high optical quality. Recently, thanks to the technical progress in laser field, transparent ceramic materials can be used for scintillators. In the present talk, we will introduce recent R&D topics of transparent ceramic scintillators.

9:00 AM

(GFMAT-157-2019) Analysis of the energy transfer processes in orthosilicate scintillators using transient absorption spectroscopy (Invited)

M. Koshimizu*[1]; Y. Muroya[2]; S. Yamashita[3]; H. Yamamoto[4]; T. Yanagida[5]; Y. Fujimoto[1]; K. Asai[1]

1. Tohoku University, Department of Applied Chemistry, Japan
2. Osaka University, Japan
3. University of Tokyo, Japan
4. National Institute for Quantum and Radiological Science and Technology, Japan
5. Nara Institute of Science and Technology, Japan

The development of novel scintillators with high light yields is of considerable interest. Most scintillators are composed of insulator hosts with dopants as luminescence centers. Ce^{3+} has been used as the luminescence center of various scintillators because of its fast emission due to the allowed 5d–4f transition; in these scintillators, rare-earth orthosilicates have long been used as hosts. It is widely known that the scintillation light yields are significantly different for rare-earth orthosilicates composed of different rare-earth elements. Judging from similar luminescence quantum efficiencies of Ce^{3+} ions, the difference is attributed to the difference in the energy-transfer efficiency from the host to the Ce^{3+} ions. In this study, the energy transfer from the host to the Ce^{3+} ions is analyzed by transient absorption spectroscopy using pulsed electron beams.

9:30 AM

(GFMAT-158-2019) Luminescence properties of organic-inorganic layered perovskite-type compounds under UV and X-ray irradiation (Invited)

N. Kawano*[1]; M. Koshimizu[2]; A. Horiai[2]; F. Nishikido[3]; R. Haruki[4]; S. Kishimoto[4]; K. Shibuya[6]; Y. Fujimoto[2]; T. Yanagida[5]; K. Asai[2]

1. Akita University, Japan
2. Tohoku University, Department of Applied Chemistry, Japan
3. National Institute of Radiological Sciences, Japan
4. High Energy Accelerator Research Organization, Japan
5. Nara Institute of Science and Technology, Japan
6. University of Tokyo, Japan

The effects of organic moieties on the scintillation properties of organic–inorganic layered perovskite-type compounds have been investigated. Three kinds of single crystals were fabricated, namely, $(C_4H_9NH_3)_2PbBr_4$ (C4), $(C_6H_5CH_2NH_3)_2PbBr_4$ (Ben), and $(C_6H_5C_2H_4NH_3)_2PbBr_4$ (Phe). Among the single crystals, the light output of Phe was found to have the greatest value when exposed to X-ray radiation (67.4 keV). The light output of Phe was 0.62 times that of YAP:Ce. The relative values of the light outputs among the fabricated single crystals under X-ray radiation correlated well with those of the quantum efficiencies and the luminescence intensity under ultraviolet radiation.

10:20 AM

(GFMAT-159-2019) Photoluminescence and Scintillation in New Oxyfluoride Glasses with Designed Fluoride Segregation (Invited)

K. Shinozaki*[1]; S. Sukenaga[2]; H. Shibata[2]; K. Ohara[3]; G. Okada[4]; N. Kawaguchi[5]; T. Yanagida[5]

1. AIST, Inorganic Functional Materials Research Institute, Japan
2. Tohoku University, Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Japan
3. JASRI, Japan
4. Kanazawa Institute of Technology, Japan
5. Nara Institute of Science and Technology, Graduate School of Materials Science, Japan

Transparent phosphors are key materials for lasers, sensors, amplifiers, and lightings. Fluorides are attractive host materials for RE^{3+}-based phosphors because of their low phonon energy, large RE^{3+} solubility, low melting temperature, and wide transparent wavelength region. Fluoride glasses, however, have poor water resistance and high mechanical brittle nature. In this work, we realized a highly efficient photoluminescent glasses by fabricating fluoride rich segregation in oxyfluoride glasses by material design. We synthesize new fluoroborate-based glasses such as BaF_2-Al_2O_3-B_2O_3 with a high fluorine content. Glass structural analyses and MD simulation indicated that the glasses form fluoride-rich segregation. The Eu^{3+}-doped glasses showed an excellent luminescence with extremely high quantum yield of 97 % in the visible region at the excitation of near UV light. Scintillation characteristics of glasses were also investigated. The glass with Ce^{3+}-doping showed good characteristics of detecting gamma rays and neutron rays among glasses.

10:50 AM

(GFMAT-160-2019) Fluoride Scintillators for Thermal Neutron Detection (Invited)

N. Kawaguchi*[1]; T. Yanagida[2]

1. Nara Institute of Science and Technology, Graduate School of Materials Science, Japan
2. Nara Institute of Science and Technology, Japan

Neutron scintillators containing ^{6}Li, ^{10}B or Gd elements emit light by excitation energies generated from nuclear reactions between these elements and thermal neutrons. The ^{6}Li-based materials are widely used for this application due to the high excitation energy by the $^6Li(n,\alpha)^3H$ reaction (Q=4.8 MeV). Most of lithium compounds show hygroscopicity, and conventional neutron scintillators with high light yields are also hugely hygroscopic (e.g., LiI:Eu and Cs_2LiYCl_6:Ce). On the other hand, the lithium fluoride and many Li containing complex fluorides are non-hygroscopic. In the past few years, we have studied scintillation properties of various fluoride-based non-hygroscopic phosphors for thermal neutron detection (e.g., LiF:W, LiF/CaF_2:Eu eutectic, $LiCaAlF_6$:Ce and $LiCaAlF_6$:Eu). In this presentation, we will introduce these results.

G4: Porous Ceramics for Advanced Applications through Innovative Processing

Porous Bioceramics I

Room: Trinity III
Session Chair: Manabu Fukushima, National Institute of Advanced Industrial Science and Technology (AIST)

8:30 AM

(GFMAT-161-2019) Unidirectional oriented Porous Ceramic and Zirconia with bioactive surface (Invited)

G. Turri*[1]; H. Muto[2]

1. Namiki Precision of Europe SA, Business and R&D Division, Swaziland
2. Adamant Namiki Precision Jewel Co., Ltd., Advanced R&D Dept, Japan

Adamant-Namiki contributes to changing the lifestyle by developing Only-one products and combining our core technology with our newest development, among which is worth mentioning high-performance ceramic products and state-of-the-art precision machining techniques. In this presentation, we will report "Unidirectional oriented Porous Ceramic" and "Zirconia with bioactive surface", two of our newes technology development. Porous Ceramics prepared by our new technique have high elastic properties due to the structural rigidity combined with unidirectional oriented porosity. Our zirconia with bioactive surface shows excellent bioactivity, confirmed by the immersion into simulation body fluid (SBF), together with high mechanical properties, compared to those of conventional commercial zirconia based-materials. Furthermore, the shape-forming can be conveniently and arbitrarily achieved by our original manufacturing method, thus providing flexibility for newer applications. We will conclude reporting on the "Zirconia Disc for Dental", which is one of our products with distinctive characteristics.

9:00 AM

(GFMAT-162-2019) Fabrication and Characterization of Hydroxyapatite/Poly(lactic acid) Porous Scaffolds (Invited)

S. Kobayashi*[1]; Y. Zusho[1]; T. Osada[1]

1. Tokyo Metropolitan University, Mechanical Engineering, Japan

In the present study, hydroxyapatite/poly(lactic acid) porous scaffold for bone tissue engineering was fabricated and characterized. At first, porous hydroxyapatite with the uniform arrangement of pore channels was obtained by forming ice crystals with in a gel containing dispersed hydroxyapatite particles, followed by sublimation of the ice under vacuum and subsequent sintering. The porous hydroxyapatite scaffold obtained was immersed in the poly(lactic acid) solution. The coated scaffold was dried in an oven. Compression tests were conducted on the specimen fabricated. Compressive modulus and strength for the coated scaffold were improved by 71 % and 82 %, respectively comparing to the non-coated scaffold.

9:30 AM

(GFMAT-163-2019) Porosity of calcium phosphate ceramic granules and ceramic-collagen composites used as bone void fillers (Invited)

I. R. Dunkley*[1]; K. Nieder[1]

1. Medtronic, Biologics, USA

The application of resorbable calcium phosphate ceramics as bone void fillers and autologous bone graft extenders for skeletal reconstruction in clinical practice is well established. Commercially available in granule forms or combined with a carrier into preformed shapes, these implantable devices provide an osteoconductive surface to support new bone growth and are resorbed and replaced during natural healing. The porous architecture of these devices influences their ability to be incorporated into the implantation site as well as the remodeling rate, and is therefore, a critical feature of the device design. By forming large interconnected pores into the ceramic structure, devices may be designed to facilitate cell and vascular infiltration throughout the bulk of the construct upon implantation while also providing room for immediate bone deposition and the development of marrow space. The devices may also be engineered with a micro-scale architecture to enhance cell seeding, migration, and response. Consequently, characterization of both macropore and micropore scale features, in addition to measuring total porosity, is necessary to predict how these materials will perform upon implantation. Here, recent benchtop, in vitro and in vivo studies performed to characterize the porosity of commercial resorbable ceramics are presented.

High SSA Ceramics

Room: Trinity III
Session Chairs: Young-Wook Kim, University of Seoul; Kay Teraoka, National Institute of Advanced Industrial Science and Technology (AIST)

10:20 AM

(GFMAT-164-2019) Microwave-emulsion method for the fabrication of spherical mesoporous silica-titania (Invited)

M. Inada*[1]; J. Hojo[2]

1. Kyushu University, Center of Advanced Instrumental Analysis, Japan
2. Kyushu University, Faculty of Engineering, Japan

Microwave process has been developed as one of hydrothermal processes for synthesis of fine oxide particles. The noteworthy phenomenon of microwave irradiation is the selective heating of high-dielectric solvent. Microemulsion method is useful to synthesize spherical oxide particles. In this study, we synthesized spherical mesoporous silica and silica-titania particles by sol-gel method using W/O emulsion under microwave irradiation, in which the oil phase does not absorb microwave, whereas the water phase is selectively heated under microwave irradiation. W/O emulsion was prepared by mixing partially hydrolyzed $Si(OC_2H_5)_4$ aqueous solution including C_{18}TAC as template with n-hexane solution including polyglycerol polyricinalate as emulsifier. In SiO_2-TiO_2 system, $TiOCl_2$ was added to the aqueous phase as TiO_2 source. We can obtain the spherical mesoporous silica and silica-titania in all cases. The specific surface area and pore size of spherical products were 800 m^2/g and 1.6 nm, respectively, which indicates that the spherical products have mesoporous structure. These results suggest that sol-gel reaction in water phase proceeds rapidly because microwave quickly and selectively heats up the aqueous solution. Photocatalytic property was investigated by the degradation of MB under UV irradiation.

10:50 AM

(GFMAT-165-2019) Interior Porosity Designed Synthesis of Mesoporous Alumina Powders Using Polymeric Surfactants (Invited)

T. Kimura*[1]

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

Surfactant assisted synthesis of ordered mesoporous materials has often been important for providing porous ceramics that potentially possess a wide variety of unique properties due to their structural features such as high surface area and large pore volume. However, except for silica and carbon, it is quite difficult to design such porous structures for non-silica-based metal oxide powders because corresponding precursors like metal alkoxides are awfully reactive in the presence of water and then precipitated before the formation of ordered mesostructures. In this presentation, I'd like to introduce our aerosol-assisted strategy to obtain alumina powders having designed interior porosity as a series of highly porous catalytic supports by applying the synthetic methods of mesoporous alumina films using polymeric surfactants. In the case using $EO_nPO_mEO_n$, we succeeded in preparing alumina powders having exceptional high surface area (about 540 m^2 g^{-1}) by improving the connectivity of mesopores

(~ 5 nm) with controlled swelling of aromatic compounds. Expansion of mesopores was also possible by utilizing PS-b-PEO. The pore dimeter was roughly estimated to be ~ 25 nm (~ 240 $m^2 g^{-1}$) and increased up to 40 nm and larger by adding PS homopolymers. These insights will be practically useful as a facile approach for preparing high-quality porous powders composed of various metal oxides.

11:20 AM

(GFMAT-166-2019) Formation of electrospun nanofibers with nanobelt, hollow and lamellar morphologies (Invited)

G. Grader*[1]; O. Elishav[2]; Y. Shener[1]; V. Beilin[1]; G. S. Shter[1]

1. Technion - Israel Institute of Technology, Chemical Engineering, Israel
2. Technion - Israel Institute of Technology, Israel

Ceramic nanofibers with designed morphology, chemical and physical properties are highly desirable for the development of advanced materials. Electrospinning is a simple approach to produce polymer, ceramic and composite nanofibers of various materials. In ceramic nanofibers the electrospinning stage is typically followed by thermal treatment to remove the polymer and obtain the final structure and phase. This step often includes shrinkage, deleterious deformation, and phase and morphology changes. One of the most important aspects of ceramic nanofibers is their final morphology. Hollow nanofibers, nanobelts and mesoporous fibers receive significant attention due to their superbly high area to volume ratio. The effect of electrospun precursor composition, mat thickness and heating rate was found to alter the final morphology from solid nanofibers to nanobelts or hollow nanofibers. With a certain mat thickness, overheating is observed altering the final obtained morphology. The morphology transformation mechanism governing the formation of hollow nanofibers, nanobelts and lamellar structures as a function of thickness, composition and heat rate is discussed. The obtained results are useful for reproducible production of nanofibers with controlled morphology.

11:50 AM

(GFMAT-167-2019) Enzyme-modified ceramic capillary membranes for the production of peptides under flow

M. M. Hoog Antink*[1]; T. Sewczyk[2]; S. Kroll[3]; P. Árki[4]; S. Beutel[2]; K. Rezwan[1]; M. Maas[1]

1. University of Bremen, Advanced Ceramics, Germany
2. Leibniz University Hannover, Institute for Technical Chemistry, Germany
3. University of Applied Sciences and Arts, IfBB – Institute for Bioplastics and Biocomposites, Germany
4. Technische Universität Bergakademie Freiberg, Institute of Electronic and Sensor Materials, Germany

In this study, we investigate the effect of membrane surface functionalization on the immobilization of the enzyme subtilisin A and its performance in the production of peptides from the model protein casein under flow. The surface of macroporous yttria stabilized zirconia capillaries was silanized with (3-aminopropyl)triethoxysilane (APTES) and 3-(triethoxysilyl)propylsuccinic anhydride (TESPSA), which served as enzyme linkers. The amount of immobilized subtilisin correlated with electrostatic interactions between the enzyme and the capillary supports. Enzyme leaching was decreased by covalent binding. It was minimal for subtilisin covalently bound to TESPSA and only slightly improved by binding to APTES over adsorptive binding to non-functionalized reference capillaries with native hydroxyl groups. Preferred enzyme orientation might have caused a more than 5 times higher specific activity of immobilized subtilisin on hydroxylated and aminated substrates compared to carboxylated surfaces. Differences in surface-enzyme interactions were also reflected by variations in peptide composition after protein hydrolysis. Accordingly, we demonstrate that surface functionalization critically determines the surface properties of ceramic enzyme supports in the production of peptides under flow and allows tailoring the performance of enzyme-modified ceramic membranes.

Innovative Characterization and Behavior of Porous Ceramics

Room: Trinity III
Session Chair: Mary Anne White, Dalhousie University

1:30 PM

(GFMAT-168-2019) Three-dimensional flow in the pores of the porous material can be evaluated using the micro X-ray CT image (Invited)

N. Nango*[1]; K. Nomura[1]; Y. Horiguchi[1]; S. Kubota[1]

1. RATOC SYSTEM ENGINEERING CO., LTD, Japan

Porous materials are used in many fields. Artificial bone is a passageway of bone-related cells and a scaffold for cells to form bone. Also, the exhaust filter of automobiles has catalytic action and filters harmful substances contained in gas. It is necessary to predict whether porous materials can match individual needs. Conventionally, a mercury penetration method has been used for pore evaluation of a porous material. In this, although the pore size distribution can be obtained, the network constituting the pores, the distribution of pressure and flow can not be predicted. Three-dimensional fluid simulation analysis is also used, but the calculation cost is high. In this study, X-ray CT scan was performed on the porous materials to calculate the structure index of the pores. We approximated the actual pore structure with a pipe network to create a pore structure model. In addition, the inlet and the outlet were given to the porous structure, the flow resistance was defined in the pores, pressure was applied between the inlet and the outlet, and the flow in the pipe network was simulated three-dimensionally. By this simulation, it was possible to realize the porous material model and to obtain the structure and flow index of the porous material with high accuracy within a practical time. The results of the flow simulation correlated with the fluid simulation analysis.

2:00 PM

(GFMAT-169-2019) Resilient ceramic aerogels constructed by silicon-based nanowires (Invited)

H. Wang*[1]; L. Su[1]; M. Li[1]; D. Lu[1]

1. Xi'an Jiaotong University, Material Science and Engineering, China

The low density, high porosity, large surface area and chemical stability are typical characteristics of ceramic aerogels, which leads to their novel applications as thermal insulators, catalyst supports, filters and hosts for functional materials. However, conventional ceramic aerogels are usually constructed by oxide nanoparticles. Brittle nature and volume shrinkage of the oxides at elevated temperature (e.g., 600 °C for silica) are limitations for their practical applications. Here we chose one dimensional nanoscale building blocks, SiC nanowires and Si_3N_4 nanobelts, to construct SiC and Si_3N_4 aerogels, via a facile one-step CVD method. The nanowire-assembled aerogels exhibit fascinating properties of ultralow density (1~10 mg/cm^3), large strain resilient compressibility (40~80%), high-temperature resistance (>900 °C in ambient air and >1500 °C in argon), and excellent thermal insulation performance (~0.02 W/mK). In particular, the Si_3N_4 aerogel exhibits high electronic wave-transparency (dielectric constant of 1~1.04 and dielectric loss of 0.001~0.004). These properties are originated from the well-interconnected highly porous 3D architecture, and superior mechanical, chemical and physical nature of the nanowires. The successful fabrication of the aerogels may provide new insights into the development of ceramics in a lightweight, resilient, and multi-functional form.

2:30 PM

(GFMAT-170-2019) Effect of porous C/C preforms density on water lubrication tribology properties of C/C-SiC composites fabricated by RMI

J. Wang*[1]; X. Liu[1]

1. Xi'an Jiaotong University, School of Materials Science and Engineering, China

Four types carbon fiber reinforced SiC matrix(C/C-SiC) composites are fabricated by porous C/C composites via reactive melt infiltration, while porous C/C composites prepared through chemical vapor infiltration(CVI). Tribology property of C/C-SiC composite are measured under simulated water lubrication conditions. The result show that it is the porosity of C/C composites that limit SiC formation in the C/C-SiC composites with same fiber volume fraction. The friction coefficient of the C/C-SiC composite is not only influenced by the load but also impacted by the content of SiC. Friction coefficients of the C/C-SiC composites first go up and then fall down as the load/SiC content increases and are much smaller compare with friction coefficient under dry condition. It is water and friction film that plays an important role in decreasing friction coefficien. The surface microstructure and wear debris on wear-induced surfaces of C/C-SiC composites disks are investigated by LSCM and SEM. The friction surface and wear debris results indicate that the main wear mechanism of C/C-SiC composite is the grain-abrasion.

2:50 PM

(GFMAT-171-2019) Sol-gel oxycarbide derived carbons developed through chemical and chlorine etching and their electrochemical characteristics

A. Tamayo*[1]; M. Rodriguez[2]; L. Salvador[2]; F. Rubio[1]; A. Mazo[1]; J. Rubio[1]

1. Institute of Ceramics and Glass, CSIC, Spain
2. University of Extremadura, Spain

There is no doubt that the full implementation of sustainable energy sources will be accompanied by the development of green batteries, capacitors and fuel cells to respond to the energy needs in a highly demanding society. Advances in supercapacitors are delivering better-than-ever energy-storage options and, in some cases, they can compete against more-popular batteries in a range of markets. A variety of electrode and electrolyte materials are possible, being the carbon (nano)materials among the top choices as electrodes for energy storage applications owing to their versatile structures ranging from 0D to 3D and tunable surface chemistry. We have synthesized sol-gel derived silicon oxycarbide materials containing different carbon contents and metal oxides as well to produce the corresponding (oxy)carbide derived carbons after chemical and chlorine etching. The carbon nanostructures developed after the treatment have been characterized through spectroscopic techniques. The surface characteristics as well as their textural properties have been obtained and correlated with their electrochemical performance for being used in double layer capacitors.

Mechanical and Thermal Properties of Porous Ceramics

Room: Trinity III
Session Chair: Satoshi Kobayashi, Tokyo Metropolitan University

3:20 PM

(GFMAT-172-2019) Processing of High Strength Porous Silica Ceramics with Low Thermal Conductivity (Invited)

Y. Kim*[1]; S. Rajpoot[1]; R. Malik[1]

1. University of Seoul, Dept. of Materials Science & Engineering, Republic of Korea

Porous ceramics have received significant attention in the field of thermal–insulation applications. However, their poor mechanical strength often limits their structural applications. In this study, the effects of polysiloxane addition on thermal conductivity and mechanical properties of porous silica ceramics were investigated. As the sintering temperature increased from 600 ºC to 800 ºC, the compressive strength increased from 3.9 MPa to 11.1 MPa in porous silica ceramics without polysiloxane addition. For the specimens containing polysiloxane, the compressive strength increased from 10.7 MPa to 14.5 MPa with increasing the sintering temperature from 600 to 800 ºC owing to: (1) decreased porosity and pore size from 73.3% to 71.3% and from 97 nm to 70 nm because of enhanced densification, respectively; and (2) formation of polysiloxane-derived SiOC, which acted as a strong bonding phase between the fumed silica particles. The thermal conductivity of the porous silica ceramics increased from 0.044 $Wm^{-1}K^{-1}$ to 0.062 $Wm^{-1}K^{-1}$ with increasing the polysiloxane content from 0 to 20 wt% when sintered at 600 ºC. The porous silica ceramics exhibited high insulation performance (0.044–0.085 $Wm^{-1}K^{-1}$) with excellent compressive (3.9–14.5 MPa) and flexural (0.47–1.04 MPa) strengths.

3:50 PM

(GFMAT-173-2019) Thermal Properties of Freeze-Cast Ceramics (Invited)

M. White*[1]

1. Dalhousie University, Canada

The freeze-casting process allows control of morphology and properties of porous materials. We have used such control to influence thermal properties of materials. Our recent investigations concerning thermal expansion and thermal conductivity will be presented.

4:20 PM

(GFMAT-174-2019) Research on porous ceramics for heat-insulation (Invited)

C. Wang*[1]

1. Tsinghua University, China

With the development of aerospace industry, higher requirements, e.g. lightweight, high temperature resistance, high strength and low thermal conductivity, have been put forward for heat insulation materials for high temperature parts. The properties of porous ceramics depend on the characteristics of the composition and structure including porosity, pore configuration, pore size and distribution. In this presentation, some progress on porous ceramics for heat-insulation in my group will be reported. Some novel processing techniques, including modified gelcasting, freeze-casting, fiber reinforcing, aerogel impregnation, hollow-grained processing and so on, have been developed to design and control the specific porous structure, therefore, some specific properties including ultra-high porosity, ultra-lightweight, high strength, and low thermal conductivity have be achieved for some potential heat-insulation applications. The matching relationship between strength and thermal conductivity will also be discussed.

4:50 PM

(GFMAT-175-2019) Thermal conductivity using three-dimensional oriented microstructures in gelation freezing derived cellular ceramics

M. Fukushima*[1]; H. Hyuga[1]; Y. Yoshizawa[1]

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

Thermal conductivity of unidirectional cellular ceramics prepared by gelation freezing route was simulated using actual three-dimensional (3D) models, collected by X-ray computed topography. Homogenization method was firstly analyzed by the 3D microscopic models, the temperature variation in macroscopic models, comprised of the microscopic models was simulated by the finite element method (FEM), and the local heat conduction in the microscopic models was again analyzed. Those simulated results were well consistent with the experimental results. This proposed strategy based on actual microstructures is expected as a promising approach to predict various thermal properties of porous ceramics in various scales.

5:10 PM

(GFMAT-176-2019) Young's modulus and Poisson's ratio of porous ceramics with random microstructure

W. Pabst*[1]; T. Uhlirova[1]; E. Gregorova[1]

1. University of Chemistry and Technology, Prague, Department of Glass and Ceramics, Czechia

The porosity dependence of Young's modulus has been a mainstay of ceramic research for many decades, so that satisfactory predictions are available for many types of microstructures (a prominent exception being partially sintered ceramics, for which this problem of parameter-free predictions has remained largely unsolved so far). However, it has to be recalled that even isotropic materials have two independent elastic constants. The porosity dependence of other elastic constants is much less predictable than that of Young's modulus, and in particular predicting the porosity dependence of Poisson's ratio is an intricate problem for which no simple solution is available. This contribution summarizes recent results concerning the porosity dependence of Young's modulus and recalls the micromechanical model predictions that are currently available for the Poisson ratio of porous materials. In the second part of the present contribution the analytical model predictions are confronted with results of numerical calculations obtained for various digital random model microstructures (isolated or overlapping spherical pores, concave pores between overlapping solid spheres, open and closed-cell foams). It is shown that for convex pores both our results are very close to those of Roberts and Garboczi, whereas for foams as well as partially sintered ceramics our results seem to be more realistic.

G6: Multifunctional Coatings for Sustainable Energy and Environmental Applications

Thick Films and Coatings for Energy Applications

Room: Trinity II
Session Chairs: Kentaro Shinoda, National Institute of Advanced Industrial Science and Technology (AIST); Tetsuya Yamamoto, Korea University of Technology

8:30 AM

(GFMAT-177-2019) Agglomeration of suspended solids in suspension plasma spraying (SPS) Process (Invited)

J. Mostaghimi*[1]; E. Dalir[1]; M. Javid[1]; A. Dolatabadi[2]; C. Moreau[2]

1. University of Toronto, Mechanical and Industrial Engineering, Canada
2. Concordia University, Mechanical and Industrial Engineering, Canada

Suspension plasma spray is a process where the micron-size feedstock is dispersed in a liquid before sprayed into a plasma jet. Problems related to the injection of fine powders are thus avoided. Deposition of such fine powders translates into a finer microstructure of the coating. Understanding how suspended droplets breakup, evaporate and agglomeration of the fine powder is of fundamental importance to the process. An accurate model of this process includes the development of a realistic model of the plasma fields both within and outside of the torch. A three-dimensional, time-dependent turbulent flow model to simulate the plasma fields within and outside of a DC plasma torch, is described. The model includes voltage fluctuations which has an important effect on droplet trajectories and thermal history. The interactions of spray droplets with the plasma jet is then presented. The model is capable of predicting agglomerated particle size distribution at the substrate. To understand how individual droplets interact with plasma, the details of the interaction of a single droplet injected into an RF inductively coupled plasma (ICP) is investigated. Individual droplets are injected centrally into the RF-ICP and are deposited on a substrate. Different structures of the deposits are observed and a detailed model of the evaporation of the liquid and formation of molten zirconia droplets are presented.

9:00 AM

(GFMAT-178-2019) Advanced opportunities for fine ceramic coatings and coatings properties

M. Shahien*[1]; K. Shinoda[1]; M. Suzuki[1]; J. Akedo[1]

1. National Institute of Advanced Industrial Science and Technology (AIST), Advanced Coating Technology Research Center, Japan

Ceramic coatings had been implemented in wide range of industrial applications to overcome the problems of corrosion, insulation, wear, and friction, as well as to increase the parts lifetime and to improve the surfaces appearance. Deposition of fine ceramic coatings is a promising solution to enhance the coating microstructure and its properties. However, the poor rheological properties, low flowability, and easy agglomeration of the fine powders limited its applicability in different coating techniques such as thermal spraying. In advanced coating technology research center (ACT) of AIST, we are focusing on fine ceramic particles deposition via several spraying techniques. This study will introduce some of our advanced development for fine ceramics spraying. Several fine ceramic coatings were successfully fabricated by plasma-assisted aerosol deposition (so called hybrid aerosol deposition; HAD), a newly developed dc plasma spraying system and axial suspension plasma spraying (ASPS). In addition the properties of the fabricated coatings will be discussed in details.

9:20 AM

(GFMAT-179-2019) Toward Reducing the Environmental Footprint in the Manufacture of Plasma Sprayed YSZ Thermal Barrier Coatings (TBCs) (Invited)

R. S. Lima*[1]

1. National Research Council of Canada, Canada

Since the 1970s the Ar/H_2 plasma has been the standard air plasma spray (APS) gas system employed to deposit ZrO_2-Y_2O_3 (YSZ) TBCs for the gas turbine industry. Although yielding higher YSZ deposition efficiency (DE) levels, N_2/H_2 plasmas did not become the main stream plasma system. This N_2/H_2 issue occurred due to problems like preliminary torch Cu-nozzle erosion and the tendency to produce denser coatings; potentially leading to TBCs exhibiting higher thermal conductivity (TC) and lower thermal cycle lifetimes. However, in the 21st century, environmental/economical impacts are becoming paramount. In addition, the introduction of new technologies (e.g., particle T & V sensors) has increased dramatically the stability and reproducibility of APS processing. A commercial YSZ feedstock was sprayed using a legacy APS torch, employing Ar/H_2 and N_2/H_2 plasmas. The top-performing Ar/H_2 and N_2/H_2 TBCs exhibited nearly-equivalent thermal cycle lifetimes and similar TC values at RT and 1200°C. In addition, the top-performing N_2/H_2 TBC exhibited a 100% improvement in DE when compared to the top-performing Ar/H_2 TBC. These initial results show that under optimized spray conditions, N_2/H_2 TBCs have the potential to simultaneously (i) minimize production costs, (ii) increase productivity, (iii) reduce environmental footprint and (iv) meet Ar/H_2 TBC specs.

9:50 AM

(GFMAT-180-2019) Crystal structure and thermal conductivity of cation-deficient perovskite type oxides

S. Kitaoka*[1]; T. Matsudaira[1]; N. Kawashima[1]; T. Ogawa[1]; C. Fisher[1]; T. Kato[1]; D. Yokoe[1]; Y. Habu[2]

1. Japan Fine Ceramics Center, Japan
2. TOCALO Co., Ltd., Japan

Cation-deficient perovskite type oxides of the form RTa_3O_9 (R: rare-earth element) are receiving considerable attention as new thermal barrier coating materials because of their low thermal conductivities. In this study we synthesized RTa_3O_9 (R: Y, La, and Yb) powders by a urea hydrolysis method, followed by pressureless sintering, and investigated the mechanisms behind their low thermal conductivities by performing Rietveld analysis, microstructure analysis using transmission electron microscopy and first-principles molecular dynamics calculations. The crystal structures of $LaTa_3O_9$ and $YbTa_3O_9$ are tetragonal (P4/mmm) at all temperatures. In contrast, that of YTa_3O_9 changes from orthorhombic ($P2_1am$) to P4/mmm above 400°C. Because thermal conductivities of $YbTa_3O_9$ and YTa_3O_9 were extremely lower than that of $LaTa_3O_9$, thermal conduction behavior was considered to depend on ion radius of the R species more strongly than the atomic weight. The nano-sized domains that correspond to regions with different orientations of Ta-O_6 octahedral tilting tend to form in crystals with smaller R ion radii. Therefore, the formation of nano-domain boundaries, together with the high concentration of intrinsic R vacancies, appears to be largely responsible for the very low thermal conductivities of $YbTa_3O_9$ and YTa_3O_9.

10:30 AM

(GFMAT-181-2019) Tailoring the wettability of hydrophobic ceramic coatings fabricated by the solution precursor plasma spray process (Invited)

T. W. Coyle*[1]; P. Xu[2]; J. Mostaghimi[2]

1. University of Toronto, Materials Science and Engineering, Canada
2. University of Toronto, Mechanical and Industrial Engineering, Canada

Surface topography and structure have a significant effect on wettability. In this work, hydrophobic Yb_2O_3 coatings were deposited via solution precursor plasma spray by radial injection of $Yb(NO_3)_3$ solution into the plasma jet. Coatings with different microstructures and surface topographies were fabricated by manipulating process parameters such as the torch transverse speed and solution concentration, and by post-deposition plasma exposure of the coating. Hierarchical columnar-structured coatings, columnar-structured coatings with smooth surfaces, and dense coatings with relatively flat topography were fabricated and exhibited different wetting behaviors. The coating microstructures were characterized and compared, and the wettability of coatings was characterized by measuring the static water contact angle and roll-off angle. The wetting behaviors of various coatings were correlated with different coating structures and surface topographies.

11:00 AM

(GFMAT-182-2019) Fine Powder Plasma Spraying of Alumina with Various Diameter

M. Suzuki*[1]

1. National Institute of Advanced Industrial Science and Technology (AIST), Advanced Coating Technology Research Center, Japan

It is known that size of the deposited particles affect significantly both of structure and properties of the plasma sprayed coating. Suspension plasma spray process (SPS) is one of the promising techniques to prepare the coatings composed of smaller deposits nowadays. Suspension, a mixture of finer powder with alcohol/water, is injected into plasma jet and sprayed onto thesubstrate, then the coatings are composed of smaller deposits, sub to 10 μm. However, there are some difficulties in this process (especially in its injection), since spraying materils are in liquid phase. This study is a trial to establish the process for obtaining the equivalent coatings as SPS, with spraying finer powders. In this study, finer ceramic powders with four different average diameters, 1-10 micron, were plasma-sprayed and the feasibility of finer powder as spraying material was evaluated.

11:20 AM

(GFMAT-183-2019) The Role of the Interfacial Oxide film on Cold Spayed Particle Deposition at the Interface Between an Aluminum Particle and an YSZ Ceramic Substrate (Invited)

K. Ogawa*[1]; S. Nakamura[1]; Y. Ichikawa[1]

1. Tohoku University, Fracture and Reliability Research Institute, Japan

Cold spray (CS) technique has attracted the amount of attention as one of the new solid-state deposition coating processes. The CS has superior characteristics such as almost no high-temperature oxidation during spraying and high deposition efficiency, compared to the other conventional thermal spray technique. This technique has been mainly used for metallic coatings on metallic substrates. In this study, the microscopic interfacial evaluation of cold sprayed metallic coatings and ceramic substrates was conducted using the Transmission Electron Microscope (TEM) and Scanning Transmission Electron Microscope (STEM). Furthermore, as similar to other experimental approaches, the isolated single particle deposition method was adopted to understand the situation of cold spray deposited single particle on ceramic substrates. In this study, the effect of the oxide layer at the deposition interface between an aluminum particle and an Yittria Partially Stabilized Zirconia (PSZ) substrate was discussed. As a result, an exceedingly thin interfacial layer along the bonding interface was formed. STEM-EDS elementary analysis results identified the layer as an aluminum oxide. From the results, it is thought that interfacial bonding can be caused by oxygen diffusion from PSZ substrate to Al particles.

11:50 AM

(GFMAT-184-2019) Hybrid Aerosol Deposition Process: Deposition Mechanism and Functional Design

K. Shinoda*[1]; M. Shahien[2]; J. Akedo[1]

1. National Institute of Advanced Industrial Science and Technology (AIST), Advanced Manufacturing Research Institute, Japan
2. National Institute of Advanced Industrial Science and Technology (AIST), Advanced Coating Technology Research Center, Japan

We developed a Hybrid Aerosol Deposition (HAD) process for deposition of ceramic coatings. The HAD process utilizes a mesoplasma flow, which is a transitional plasma from thermal plasma to low-pressure plasma, to enhance particle deposition for aerosol deposition. We confirmed an increase in the deposition efficiency by the mesoplasma assistance, yet the detail mechanism of the deposition has not been clarified. In this study, we have investigated the microstructure of ceramic coatings obtained through spraying of alpha-alumina fine powder in the HAD process. Transmission electron microscopy and electron energy-loss spectroscopy mapping reveal that alumina coatings consisted of alpha-alumina grains with amorphous alumina on their surfaces. The amorphous layers connected each other and formed a three-dimensional bridge structure. These results indicate that the surface of fine particles was activated by the mesoplasma flow, while the core of the particles was kept solid without melting during flight. The surface activation of particles contributed to increase their sticking probability, which resulted in the increase in the deposition efficiency and the enhancement of the capability of three-dimensional coverage. This deposition mechanism is unique and different from either melt deposition or solid consolidation. Our recent activity to design function of coatings by HAD process will also be presented.

Thin Films and Functional Coatings

Room: Trinity II
Session Chairs: Jun Akedo, AIST; Thomas Coyle, University of Toronto

1:30 PM

(GFMAT-185-2019) Pulsed Photoinitiated Fabrication of Inkjet Printed Titanium Dioxide/Reduced Graphene Oxide Nanocomposite Thin Films (Invited)

D. B. Chrisey*[1]

1. Tulane University, Physics, USA

This work reports a new technique for scalable and low-temperature processing of nanostructured TiO_2 thin films, allowing for practical manufacturing of TiO_2-based devices. Dual layers of dense and mesoporous TiO_2/graphitic oxide nanocomposite films are synthesized simultaneously using inkjet printing and pulsed photonic irradiation. Investigation of process parameters including precursor concentration (10–20 wt%) and exposure fluence (4.5–8.5 J cm^{-2}) reveals control over crystalline quality, graphitic oxide phase, film thickness, dendrite density, and optical properties. Raman spectroscopy shows the Eg peak, characteristic of anatase phase titania, increases in intensity with higher photonic irradiation fluence, suggesting increased crystallinity through higher fluence processing. Transmission and diffuse reflectance are used to determine optical band gaps of the films ranging from 2.98 to 3.38 eV in accordance with the photonic irradiation fluence and suggests tunability of TiO_2 phase composition. The studied electrical and optical properties of the light processed films show comparable results to traditionally processed TiO_2 while offering the distinct advantages of scalable manufacturing, low-temperature processing, simultaneous bilayer fabrication, and in situ formation of removable carbon nanocomposites.

2:00 PM

(GFMAT-186-2019) Thermal stability of molybdenum doped titania anatase photocatalyst for indoor building materials

V. Kumaravel*[1]; S. Mathew[1]; J. Bartlett[1]; S. C. Pillai[1]

1. Institute of Technology Sligo, Nanotechnology and Bio-Engineering Research Group, Department of Environmental Science, Ireland

The commercialization of photocatalysis has received significant interest in the 21st century owing to its numerous eco-friendly applications under light irradiation. A high temperature stable titania (TiO_2) anatase is a prerequisite to fabricate ceramics and tiles with photocatalytic features for indoor air purification and antimicrobial applications. TiO_2 anatase is thermodynamically unstable at high processing temperatures and it would be transformed into TiO_2 rutile over 600 °C. Metal doping is one of the cost-effective approaches to control the anatase to rutile phase transition (ART) of TiO_2. In this present work, the ART of molybdenum-doped TiO_2 nanoparticles (Mo-TiO_2) were investigated systematically in the temperature range of 500 °C - 900 °C. Mo-TiO_2 nanoparticles were prepared via a convenient sol-gel procedure. The analytical techniques such as X-ray diffraction (XRD), Raman, and X-ray photoelectron spectroscopy (XPS) were used to investigate the phase transformation of Mo-TiO_2. The photocatalyst with a high fraction of anatase was further characterized by photoluminescence (PL) to study the charge-carrier recombination process. XRD and Raman results showed that ART was strongly influenced by the concentration of Mo dopant. Moreover, the anatase phase of TiO_2 was well maintained about 67 % using 2 % Mo-TiO_2 at 750 °C.

2:20 PM

(GFMAT-187-2019) Fabrication of Oxide Nanostructure Gas Sensor Devises by a Simple Step MOD Method Fabrication of Oxide Nanostructure Gas Sensor Devises by a Simple Step MOD Method

T. Sugahara*[1]; L. Alipour[1]; K. Suganuma[1]

1. Osaka University, Japan

In recent years, printed electronics is one of the much attention technology intend to next generation electronics device manufacturing for mass product such as high-throughput, large-scale, and resource saving over conventional process. In the previous study, oxide nanostructure arrays growth on the silica glass substrate have been successfully synthesized by a simple solution metal organic decomposition (MOD) method. Here, we are demonstrating fabrication of MoO_3 nanorods sensor device for volatile organic compounds (VOC) gas by a simple solution MOD with printed coating process. The metal oxide gas censor shows good performance with response time and complete recovery, as well as various selectivity of VOC gas at 573 K.

2:40 PM

(GFMAT-188-2019) Flexible Oxide Thin Film Grown by Excimer Laser Assisted Metal Organic Deposition

T. Tsuchiya*[1]; Y. Uzawa[1]; T. Nakajima[1]; I. Yamaguchi[1]; J. Nomoto[1]

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

To construct low carbon society more and more in the world, it is necessary to develop a low cost and power saving process for the ceramics thin film processing. For this aim we have developed the photo-induced chemical solution process for a patterned epitaxial and flexible metal oxide thin film on organic, glass and single crystalline substrates. In this presentation, we will talk about the preparation of the flexible oxide tin films on plastic substrates. By using the PRNP process, flexible ITO thin film was prepared on glass and PET substrates at room temperature. The sheet resistance of the flexible ITO film on PET is 80Ω/sq. in N_2. In addition, for the purpose of the thick film process, we developed photo reaction of hybrid solution process (PRHS) for the thick film at low temperature. By using the process, flexible $CsVO_3$ phosphor film was produced on a PET substrate. The luminescence of the film is 2000 cd/m^2. In this case, no resin was need for the film growth. Therefore, the luminescence of the film prepared by PRHS was much higher than that of the film prepared by conventional phosphor films with resin.

3:20 PM

(GFMAT-189-2019) Smart coating process of Ga-doped ZnO films for wide applications (Invited)

T. Yamamoto*[1]; Y. Furubayashi[1]

1. Kochi University of Technology, Research Institute, Japan

We will demonstrate how to tailor carrier concentration and alignment of columnar grains with identical crystallographic orientation in polycrystalline Ga-doped ZnO (GZO) films deposited on amorphous glass substrates for wide applications. In this work, we use reactive plasma deposition (RPD) with dc arc discharge. The deposition parameters are discharge current ranging from 90 to 140 A and oxygen (O_2)-gas flow rates (OFRs) ranging from 0 to 25 sccm; The O_2 gas is introduced into the deposition chamber during film growth to control O-related point defects in grains and alignments between columnar grains. The analysis of the data obtained by plasma diagnostics with mass energy analyzer and optical emission spectroscopy (OES) and Hall effect measurements yield as follows. To tailor carrier concentration, for the applications of conductive electrodes and plasmonic materials with low optical loss in infra-red (IR) wavelength region, control of flux energies of neutral Zn atoms depending on OFR is critical. For the application of gas sensor based on GZO films with poor alignment between columnar grains, a decrease in a ratio of flux of electropositive oxygen (O^+) ions to that of neutral O atoms with an increase in OFR is essential, resulting in the suppression of surface diffusion of the O atoms. In this talk, we clarify the characteristics of arc plasma of RPD to discuss what the smart process is.

3:50 PM

(GFMAT-190-2019) Development of Infrared Sensor for Detecting Water Pollution Based on Selenide Waveguide

M. Baillieul[1]; E. Baudet[1]; E. Rinnert[2]; J. Charrier[3]; L. Bodiou[3]; F. Colas[2]; K. Boukerma[2]; P. Nemec[4]; K. Michel[5]; V. Nazabal*[1]

1. CNRS-University of Rennes 1, ISCR, France
2. IFREMER, France
3. University of Rennes 1, FOTON, France
4. University of Pardubice, Czechia
5. BRGM, France

The middle infrared (mid-IR) sensor based on evanescent wave spectroscopy is a promising analytical tool for simultaneous detection and quantification of a variety of pollutants in natural waters such as hydrocarbon compounds. Chalcogenide glasses are particularly well suited for sensing applications due to their tunable refractive index and infrared transparency. Two selenide glass targets of nominal composition $Ge_{28.1}Sb_{6.3}Se_{65.6}$ (buffer layer) and $Ge_{19.4}Sb_{16.7}Se_{63.9}$ (guiding layer) were selected for their mid-IR transparency, stability against crystallization and refractive index contrast suitable for mid-IR optical waveguiding. Infrared selenide sensor were manufactured by radiofrequency sputtering and reactive-ion etching. Functionalization of the surface of the IR selenide sensor is necessary to enable hydrocarbons detection. To evaluate the chemical functionalization of the surface of a selenide layer, attenuated total reflection spectroscopy (ATR) was performed on ZnSe prism using different polymers. Measurements were performed in water to detect aromatic hydrocarbons in a concentration range from few hundred of ppb to few ppm. These elementary bricks concerning the manufacture of the IR waveguide and its functionalization allow to open the way for IR sensors dedicated to the detection of bio-chemical molecules in water.

G7: Ceramics Modeling, Genome and Informatics

Prediction of Structure and Performance III

Room: Trinity I

Session Chair: Jian Luo, University of California, San Diego

8:30 AM

(GFMAT-191-2019) New approach to the theory of formation of high entropy alloys (Invited)

W. Ching*[1]

1. University of Missouri-Kansas City, USA

In recent year, high entropy alloys (HEA) has attracted a great attention to materials research community because of many potential new applications of this unique class of alloys. HEA consist of at least 4 or 5 transition metal elements in equal atomic components. However, the fundamental theory and computational modeling of HEA is still not fully developed. Here I propose a new approach based on the detailed evaluation of the electronic structure and bonding in HEA which is quite different from existing approaches. The idea is to build large supercells of HEA in the form of random solid solution model and calculate its electronic structure and bonding to provide critical parameters, total bond order density (TBOD) and partial bond order density (PBOD) which avoids pure geometric description. Results from several HEAs including: Co20Cr20Fe30Ni30, Co30Cr30Fe20Ni20, Co20Cr20Fe20Mn20Ni20, Al20Co20Cr00Fe20Ni20 in fcc lattice will be presented and discussed.

9:00 AM

(GFMAT-192-2019) Screening Interfaces of Energy Materials Using First-Principles Calculations (Invited)

P. Canepa*[1]

1. National University of Singapore, Materials Science and Engineering, Singapore

In 2000, during his noble prize lecture Prof. Herbert Kroemer stated "The interface is the device"; he was referring to the phenomenal success in design and application of semiconductor heterojunction devices in microelectronics. Arguably, Kroemer's statement has an ever-increasing relevance across a range of technologies far beyond transistors, where heterojunctions found their initial success. Researchers are increasingly finding that interfaces between materials represent a rich space for the exploration of exotic properties that are not present in bulk materials, such as two-dimensional electron gases (or liquids) and quantum topological states. It is clear that the importance of the interface can only grow with the evolution of modern technological applications. Simultaneously, progress in computational materials science in describing complex interfaces is critical for improving the understanding and performance of energy materials, including rechargeable batteries and catalysts. In this talk, I will elucidate how first-principles calculations, based on density functional theory, can be applied to large pools of materials to rationalize their behaviors when forming functional interfaces. Focus will be given to topical materials in rechargeable batteries, where controlling interfaces is paramount to curb degradation phenomena.

9:30 AM

(GFMAT-193-2019) First principles-based studies of finite temperature properties of complex oxides (Invited)

V. R. Cooper*[1]; K. Pitike[1]; Y. Li[2]

1. Oak Ridge National Laboratory, Materials Science and Technology Division, USA
2. Oak Ridge National Laboratory, Center for Computational Sciences, USA

Computational materials design requires knowledge of material performance under device relevant conditions. This entails an understanding of responses in specific temperature ranges; not typically accessible by 0 K-density functional theory (DFT) calculations. Unfortunately, evaluating finite-temperature behavior often requires Monte Carlo or molecular dynamics simulations employing DFT-trained models. Uncertainties in the phenomenological models, and the DFT functionals used to parameterize them, tend to result in significant deviations from experiments. I will discuss our efforts to examine the limits of DFT functionals with an eye to designing more robust, efficient approaches for studying finite-temperature, materials properties of complex oxides. I will focus on temperature-dependent phase transitions in ferroelectric oxides; employing stochastic methods to access finite-temperature properties. This work illuminates the dependence of these results on the underlying DFT exchange-correlation functional. This combined approach provides a path forward for truly first-principles design of functional materials properties under device relevant conditions. Supported by the U.S. D.O.E., Office of Science, BES, MSED (first principles calculations) and the LDRD Program of ORNL (simulations), managed by UT-Battelle, LLC, for the U. S. DOE using resources at NERSC and OLCF.

Multi-scale Modeling I
Room: Trinity I
Session Chair: Wai-Yim Ching, University of Missouri-Kansas City

10:20 AM

(GFMAT-194-2019) A Decade-Long Thrust to Compute "Grain Boundary Diagrams": From Phenomenological Models to Atomistic Simulations and Deep Learning

J. Luo*[1]

1. University of California, San Diego, USA

I will review our continuing efforts to compute grain boundray (GB) "phase" (complexion) diagrams over the past decade. First, we have developed two interfacial thermodynamic models to construct GB diagrams, including a phenomenological model to compute "GB lambda diagrams" to forecast the thermodynamic tendency for general GBs to disorder at high temperatures [see, e.g., JACerS 95:2358 (2012) for binary alloys; Acta 91:202 (2015) for ternary alloys; and Acta 130:329 (2017) for oxide ceramics] and an Ising (lattice) type statistical model to compute GB adsorption diagrams [Scripta 130:165 (2017)]. Second, we are conducting hybrid molecular dynamics and Monte Carlo (hybrid MD/MC) simulations in semi-grand canonical ensembles. Here, we computed a GB diagram for Ni-doped Mo, where we also found a first-order GB phase-like transformation that breaks the symmetry [PRL 120:085702 (2018)]. More recent hybrid MC/MD simulations computed a GB adsorption diagram with first-order GB transformations for Au-doped Si, which is supported by our prior experiment and further verified by first-principles calculations [Scripta 158:11 (2019)]. Third, our on-going studies are utilizing deep learning algorithms to greatly expand our capabilities to construct "GB diagrams" beyond that can be achieved by atomistic simulations or experiments realistically.

11:00 AM

(GFMAT-195-2019) Perspectives of ion beam application for synthesis of room temperature single electron transistors embedded in SiO_2 (Invited)

F. Djurabekova*[1]; C. Fridlund[1]; K. Nordlund[1]

1. University of Helsinki, Department of Physics, Finland

Billions of tiny computers that can sense and communicate from anywhere are coming online, creating the "Internet of Things" (IoT). As the IoT continues to expand, more and more devices need batteries and plugs. Therefore, together with improved batteries, advanced computation and communication need to be deivered at extremely low power consumption. One of the solutions is to integrate high-speed CMOS structures with Single Electron Transistors (SET) that are known as low-energy dissipation devices. Recently the possibility to use ion beam mixing combined with suitable annealing has been suggested as a possible means to synthesize individual silicon quantum dots in a silica layer, with the possibility to function as single-electron transistors. For this to work, it is necessary to have a careful control of the ion beam mixing in Si/SiO2/Si heterostructures, as well as understand the nature of not only the composition, but also the chemical modification of the SiO2 layer by the mixing with Si. We show that significant insights in the synthesizing process can be enabled by using atomistic simulations. For instance, the ion hammering effect cannot be observed in any other type of simulations. This effect distorts significantly the architecture of the structure.

11:30 AM

(GFMAT-196-2019) Effective Elastic Properties of Two-Phase Composites: Numerical Studies of the Irregular Undulated Shape of Inclusions (Invited)

R. Piat*[1]; P. Happ[1]

1. Darmstadt University of Applied Science, Germany

Particle reinforced composites are widely used in industrial applications. Elastic properties of the composite can be influenced by the orientation, volume fraction, distribution and shape of the inclusions, resulting in a composite better suited for the intended application. The aim of the proposed studies is estimation the influence of undulations on the interface between the spherical inclusion and matrix material on the resulting elastic properties of two phase composites. For this purpose, firstly the geometry of the inclusions was created numerically by using the theory of spherical harmonics. The resulting surfaces were then exported to ABAQUS to calculate the elastic properties of the two-phase composites using the FE-method. Secondly the obtained elastic moduli were compared with properties of composites including only spherical inclusions, this way finding upper and lower bounds for the elastic properties. Further comparisons were made using semi-analytical approximations e.g. Self-Consistent-, Mori-Tanaka-, Dilute-Distribution-Method. Obtained results were compared with experimental and numerical results taken from literature.

Multi-scale Modeling II
Room: Trinity I
Session Chair: Xingqiu Chen, Institute of Metal Research

1:30 PM

(GFMAT-197-2019) Effects of many body interactions in potential models for ceramics (Invited)

T. Oda*[1]

1. Seoul National University, Department of Nuclear Engineering, Republic of Korea

Molecular dynamics (MD) calculation is an important computational method for materials science and engineering. To obtain meaningful results from MD simulations, a quality potential model needs to be prepared. In this study, for several ceramics, we investigate how many-body interactions affect the quality of potential models. For many-body interactions, embedded-atom method (EAM) model and three-body interaction model are considered and added to a two-body interaction model. For ceramics, binary and ternary oxides, namely Li_2O, TiO_2 and Li_2TiO_3, are tested. Potential models are constructed by using energies, forces and stresses calculated by first-principles calculation as the reference data. It is confirmed that even a two-body interaction model can nicely reproduce the reference data and reasonably reproduce experimental data on fundamental material properties including phase transition temperatures in the case of Li_2O, which is highly ionic. However, for TiO_2 and Li_2TiO_3, which contain some covalency in the Ti-O interaction, two-body interaction model is not satisfactory and the addition of many-body interactions greatly improves the quality of potential model. We propose a systematic method to construct two-body and many-body potential models for ceramics.

2:00 PM

(GFMAT-198-2019) Alkali ions sorption in cement paste: A computational study across time and length scales (Invited)

L. Béland*[1]

1. Queen's University, Mechanical & Materials Engineering, Canada

The pores of cement paste contain a high-pH solution, that includes Ca^{2+} and alkali ions, such as Na^{1+} and K^{1+}. These alkali ions can lead to severe durability issues in concrete if they interact with reactive aggregates and form an alkali-rich gel. The presence of alkali ions also provide an opportunity to produce alkali-activated slags, a class of mortars with lower greenhouse gas footprint than traditional Portland cement. Finally, cement is a considered a prime candidate to store spent nuclear fuel, which contains significant amounts of Cs^{1+}, an alkali ion. These three issues motivated a computational study of the sorption mechanisms of the alkali ions with C-S-H and ultimately, their effect on the mechanical properties of the paste. This is technically challenging for two main reasons. First, the timescales of sorption are well out of the range of traditional atomistic methods. Second, the granular nature of C-S-H means that mesoscale mechanical properties are more relevant than those at the atomistic scale, where sorption takes place. To solve the first issue, we combine a semi-grand canonical Monte Carlo procedure to the Activation Relaxation Technique nouveau. The second issue is solved by using a multi-scale, coarse grained approach based on potentials of mean force. These two methods led to insights about atomistic and meso-scale features of alkali sorption in C-S-H.

2:30 PM

(GFMAT-199-2019) Theoretical studies on triplet-triplet annihilation based photon up-conversion in solution and solid (Invited)

Y. Shigeta*[1]

1. University of Tsukuba, Center for Computational Sciences, Japan

Recently, the triplet-triplet annihilation (TTA) based photon up-conversion (UC) process has been extensively studied as a possible device that utilizes solar power because TTA-UC generates high-energy photon emission from absorptions of lower energy photons. Thus, the investigation into design principles for developing robust TTA materials is of great importance. Since TTA-UC process is quite complicated, one should analyze a series of these processes in parallel to deeply understand the mechanism of TTA-UC. In many experiments, platinum or palladium octaethyl porphyrin (PtOEP or PdOEP) and 9,10-diphenylanthrance (DPA) have been selected as the sensitizer and emitter, respectively and achieved the high TTA-UC quantum yield (QY) (26%) in solution. The present study focuses on the clarification of TTA and triplet-triplet energy transfer (TTET) processes in both solution and solid pahse using the fragment molecular orbital (FMO) method and FMO-liner combination molecular orbital (FMO-LCAO) methods with help of Marcus theory to estimate TTA and TTET rate constants. In solution, the molecular diffusion process is the rate-limiting step, while the TTET in solids. We demonstrate the reason why a derivative of DPA exhibit higher QY compared to DPA both in these phases in view of the electronic structure and dimensionality of energy migration.

Big Data and Informatics

Room: Trinity I
Session Chairs: Jincheng Du, University of North Texas; Valentino Cooper, Oak Ridge National Laboratory

3:20 PM

(GFMAT-200-2019) Spontaneous Ferroelectric Distortion Driven Weyl Semimetal State in $HgPbO_3$

X. Chen*[1]

1. Institute of Metal Research, China

The recent discoveries of ferroelectric metal and Weyl semimetal (WSM) have stimulated a natural question: whether these two exotic states of matter can coexist in a single material or not. In light of the fact that both states are formed only in systems lacking inversion symmetry, it is conceivable that this scenario can be physically realized. This motivates us to design and realize such exotic but elusive, never been accomplished material. Here, by using first-principles calculations, we demonstrate that the experimentally synthesized nonmagnetic $HgPbO_3$ represents a unique example of such hybrid Weyl Ferroelectric semimetal. Its centrosymmetric $R\bar{3}c$ phase undergoes a spontaneous phase transition to the ferroelectric R3c structure and both phases are semimetallic. These predictions are confirmed by our neutron diffraction experiments which revel a phase transition from the high-temperature $R\bar{3}c$ phase to the low temperature polar R3c phase around 250~K. More interestingly, the ferroelectric distortion also drives HgPbO$_3$ into noncentrosymmetric Weyl semimetal state with six pairs of chiral Weyl nodes around the Fermi level. The coexistence of ferroelectricity and Weyl nodes in HgPbO$_3$ makes it an ideal platform for exploring multiphase interaction and mutual control for potential applications of integrated topotronic and ferroelectric devices.

4:00 PM

(GFMAT-201-2019) Design of lithium ion solid state electrolytes by couple atomistic simulations and experimental investigations (Invited)

J. Du*[1]

1. University of North Texas, Materials Science and Engineering, USA

Solid state electrolytes are important to the development of next generation all solid state batteries, fuel cells and sensors. In this talk, I will present our recent work on combining atomistic computer simulations and experimental investigations of lithium ion solid state electrolytes materials to understand defects, defect interactions and their effect on diffusion of lithium ions in ceramics and glass systems. Issues of diffusion anisotropy as a function of temperature and methods to improve the diffusivity by defect engineering will be discussed based systematic computer simulations. Additionally, the phase transformation and crystallization behaviors are studied by in-situ high energy X-ray diffraction coupled by molecular dynamics simulations. The second type of material is the lithium aluminum germanium phosphate (LAGP). Defect energy calculations and MD simulations were used to understand defect interactions and their effect on lithium ion diffusion behaviors.

4:30 PM

(GFMAT-202-2019) Application of Computational Thermodynamics in Solid Oxide Fuel Cell (Invited)

Y. Zhong*[1]

1. Worcester Polytechnic Institute, Mechanical Engineering, USA

High sintering and operation temperatures promote unwanted interface reactions in Solid Oxide Fuel Cell (SOFC), especially at the cathode-air-electrolyte triple phase boundary (TPB). The composition change and phase stability at TPB have been identified as the dominant mechanism for the long-term degradation, which is a critical parameter for SOFC. It is greatly needed to use the computational thermodynamics (CALPHAD) approach to investigate the phase equilibria between the cathode (perovskite) and the electrolyte (doped zirconia). The talk will cover our recent discoveries on the following topics: 1.)the TPB phase stabilities (formation of LZO and SZO); 2.)the quantitative defect chemistry analysis for perovskite; 3.) the electrical property prediction (electronic and ionic conductivity) for perovskite and zirconia; 4.)the thermomechanical properties for perovskite (CTE mismatch, chemical expansion); 5.)the reactions between cathode and gas impurities, including CO_2, SO_2, H_2O, and Cr.

5:00 PM

(GFMAT-203-2019) Machine-learning phase prediction of high-entropy alloys (Invited)

H. Zhuang*[1]; W. Huang[1]; P. Martin[1]

1. Arizona State University, USA

High-entropy alloys (HEAs) are receiving intensive attention due to their unusual properties that largely depend on the selection among three phases: solid solution (SS), intermetallic compound (IM), and mixed SS and IM (SS+IM). Here we employ machine-learning (ML) algorithms to efficiently explore the phase selection rules using an experimental dataset including 174 SS, 173 SS+IM, and 54 IM phases. We first perform ML calculations on the entire dataset with three different ML algorithms: K-nearest neighbors (KNN), support vector machine (SVM), and artificial neural network (ANN). The accuracy from both the KNN and SVM classifications is below 60%, far lower than that (~100%) of the ANN. We then focus on using ANN and find that the testing accuracies in classifying SS and IM, IM and SS+IM, SS and SS+IM reach 94%, 86%, and 80%, respectively. Our work provides an alternative route of accelerating discovery of new HEAs.

G8: Advanced Batteries and Supercapacitors for Energy Storage Applications

Cathodes: Li-ion and Na-ion Battery

Room: Salon D
Session Chair: Neeraj Sharma, University of New South Wales

8:30 AM

(GFMAT-204-2019) The Sodium Layered Oxides in Na-Batteries

C. Delmas*[1]; D. Carlier[2]; M. Guignard[3]; J. Yoshida[4]

1. CNRS-ICMCB, France
2. ICMCB, France
3. ICMCB-CNRS, France
4. Toytota Motor Europe, Belgium

In the perspective of the development of very large scale renewable energy systems the prevailing parameters are the lifetime, the price and the material availability. From these points of view, sodium based batteries have to be investigated. Our research group studied layered oxides as positive electrode for 30 years. Recently, a general investigation was undertaken with a special focus on P2-type layered phases. One of the main interests of this structure is the existence of an ion conduction plane made of face sharing trigonal prims which exhibits a high ionic diffusivity thanks to the existence of a large bottleneck (oxygen rectangle) for sodium diffusion. This structure is able to accommodate a lot of transition metal cations, allowing the optimization of the properties by cationic substitution. Studies was performed on the P2-$Na_x(Mn,Co)O_2$, $Na_x(Mn,Fe)O_2$, $Na_x(Mn,Fe,Co)O_2$ and $Na_x(Mn,Fe,Ni)O_2$ systems with various amounts of transition metal ions. All materials crystallize in the hexagonal system ($P6_3$/mmc). The comparison of their behavior with that of materials with a single transition element in the MO_2 slabs ($NaCoO_2$, $NaVO_2$) allows to evidence the relation between the sodium vacancy ordering and the cation distribution in the MO_2 slabs.

9:05 AM

(GFMAT-205-2019) Aqueous Processing and Formation of Ni-Rich Cathodes for Lithium-Ion Batteries (Invited)

D. L. Wood*[1]; M. Wood[1]; S. An[1]; J. Li[1]; Z. Du[1]; R. Ruther[1]; C. Mao[1]

1. Oak Ridge National Lab, Fuel Cell Technologies Program, USA

Ni-rich, or low-Co, layered active materials are promising candidates for next-generation cathodes for lithium-ion batteries. However, these materials present processing and performance challenges such as compatibility with water during aqueous electrode formulation, unoptimized SEI/CEI formation conditions during cell assembly, and unstable capacity fade when cycled to upper cutoff voltages above 4.3 V vs. Li/Li^+. The DOE Battery Manufacturing R&D Facility at ORNL (BMF) has recently emphasized low-Co-containing and high-energy $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC 811) to enable its use in electric vehicles. To decrease the high manufacturing cost associated with long formation times for low-Co cathodes, five different formation protocols were studied using graphite anodes where the total formation time varied from 10 to 86 h. Electrochemical characterization and post mortem analysis showed that longer formation times do not necessarily improve long-term performance while extremely short formation protocols result in lithium plating and poorer electrochemical performance. It was found that the optimum formation protocol is intermediate in length to minimize impedance growth, improve capacity retention, and avoid lithium plating. This presentation will also focus on aqueous processing conditions and other fast formation protocols that are being developed for NMC 811 and other low-Co and Co-free cathodes.

9:35 AM

(GFMAT-206-2019) DFT-assisted Solid State NMR Characterization of Vanadium Fluorophosphates as Battery Materials

D. Carlier*[1]; T. Bamine[1]; P. Sanz-Camacho[1]; L. Nguyen[1]; E. Boivin[1]; C. Masquelier[3]; L. Croguennec[2]

1. ICMCB, France
2. ICMCB-CNRS, France
3. LRCS, France

In the scope of finding new positive electrode materials for Li-ion or Na-ion batteries, the deep understanding of the link between their structure, electronic structure and electrochemical behavior is crucial. As the presence of defects or disorder may play a critical role, a local characterization of the materials is highly required. To that extent, Magic Angle Spinning Nuclear Magnetic Resonance (MAS-NMR) appeared to be a key tool. For paramagnetic materials, it allows to probe both, the local structure and the local electronic structure thanks to the Fermi contact interaction. In order to assign the signals and understand the spin transfer mechanism through the chemical bonds, we have been developed the use of ab initio calculations for some years. Some recent studies of the characterization of defects or disorder in layered oxides or V-phosphate materials will be presented. Using MAS-NMR we showed that several phosphate materials as $LiVPO_4F$, or $Na_3V_2(PO_4)_2F_3$, which are promising materials for positive electrode application in Li-ion and Na-ion batteries respectively, exhibit some O-defects leading to the formation of V^{4+} ions locally. These V^{4+} ions are forming a vanadyl-type bond with the defect O, and affect the electrochemical cycling performances.

Na-ion Battery and Capacitors

Room: Salon D
Session Chair: Dany Carlier, ICMCB

10:20 AM

(GFMAT-207-2019) Sodium reactivity in Na-Mn-O systems (Invited)

V. Pralong*[1]; E. Adamczyk[2]

1. CNRS ENSICAEN, France
2. CNRS CRISMAT, France

Among the cathodes of the sodium ion batteries, the manganese and vanadium based oxide materials present many advantages due to their high energy density, low-cost and low-toxicity. In particular, numerous layered materials have been reported in the system Na-Mn-O. These materials are interesting because they show weak interlayer interactions with free space allowing sodium diffusion. In this presentation, two different phases will be presented: $Na_4Mn_2O_5$ and $Na_2Mn_3O_7$. The Kagome network of $Na_4Mn_2O_5$ is made of layers of corner-sharing square-pyramids of MnO_5. This material was synthesized by a conventional solid-state method starting from Mn_2O_3 and Na_2O and it shows a first charge capacity of 380 mAh/g and a reversible capacity of 130 mAh/g. The reversible capacity is then improved to 220 mAh/g. $Na_2Mn_3O_7$ is obtained via a simple synthesis from cheap sodium and manganese salts, consists of Mn-vacancy-$[Mn_3O_7]^{2-}$ layers built up with edge-sharing MnO_6 octahedra, separated by NaO_6 and NaO_5 polyhedra. Starting from this phase, a reversible capacity of 2 Na/f.u. (160 mAh/g) is obtained through a plateau at 2.1 V with a low polarization of 100 mV. Interestingly, an additional reversible redox process, corresponding to the extraction of 1.5 Na^+, is observed on oxidation at 4.1 V due to the oxygen redox activity. The mechanism of extraction as well as the structures of the as-prepared and oxidized phases will be discussed in this presentation.

10:50 AM

(GFMAT-208-2019) Na-Mn-O compounds for rechargeable sodium batteries (Invited)

S. Myung*[1]

1. Sejong University, Republic of Korea

Lithium resource is not abundant element and unevenly distributed in earth. Indeed, the price of lithium has dramatically surged due to commercialization of lithium batteries for power sources of vehicles and energy storage systems. Sodium resource is possible to be compared with lithium resources as counterpart because sodium is one of the most opulent elements on the Earth. In addition, sodium is the second lightest and smallest alkali metal. Above all, intercalation chemistry of sodium is similar to lithium. For this reason, we decided to attempt to prepare distorted orthorhombic - $Na_{0.67}MnO_2$ based on $Mn^{3+/4+}$ redox reaction synthesized by spray pyrolysis. Sodium layered oxide, $Na_{0.7}MnO_2$, with the distorted orthorhombic (space group: Cmcm) type structure was synthesized by an ultrasonic spray pyrolysis method and characterized as positive electrode for sodium batteries. The $Na_{0.67}MnO_2$ electrode delivered a high specific capacity of 228 $mAhg^{-1}$ at 0.05C rate in the 1.5–4.3 V range. The capacity retention after 50 cycles is about 75% in the 1.5–4.3 V range. This reason of high capacity retention would be structural stability of the distorted orthorhombic $Na_{0.67}MnO_2$ electrodes during cycling. Details will be discussed in the in the meeting.

11:20 AM

(GFMAT-209-2019) Lithium and sodium electrochemical (de) intercalation in layered molybdenum oxides (Invited)

M. Guignard*[1]; M. Suchomel[1]; N. Sharma[2]; C. Delmas[1]

1. ICMCB-CNRS, France
2. University of New South Wales, Australia

Lithium and sodium layered oxides, with the general chemical formula A_xMO_2 (A: Li or Na, M: transition element and $0 \le x \le 1$), have been studied for 30 years to be used as positive electrode materials in lithium-ion or sodium-ion batteries. Whereas systems containing 3d elements have been intensively studied, systems with 4d transition metal ions have been less investigated due the high molecular weight of 4 d elements. We will present first the phase diagram of the system Na_xMoO_2 which has been studied using electrochemistry combined with in situ synchrotron X-ray diffraction experiments. The many steps observed in the electrochemical curve of $Na_{2/3}MoO_2$ during cycling in a sodium battery suggest numerous reversible structural transitions during sodium (de)intercalation $Na_{0.5}MoO_2$ and $Na_{\sim 1}MoO_2$. We will present finally the first results that were obtained in the system Li_xMoO_2. It has also been studied using electrochemistry combined with in situ laboratory X-ray diffraction experiments. Even if the phase diagram in the Li_xMoO_2 is less complicated than that of the Na_xMoO_2 system, many phase transitions still occur in during the lithium electrochemical (de) intercalation. The large number of phase transitions is usually not observed in lithium layered oxides containing 3d elements, indicating the molybdenum tends to rearranges within the $[MoO_2]$ layers.

11:50 AM

(GFMAT-210-2019) High Permitivity Ceramics for Single Layer Capacitors and Energy Storage Devices

V. Krstic*[1]

1. Functional Materials Manufacturing Inc., Canada

Due to ever increasing demand for energy storage and its transport, there is a need for a new generation of materials and devices capable of storing large amount of electric energy without problems associated with disposal and environmental pollution. Historically, the liquid-electrolyte batteries have been the most common way of storing electrical energy. However, this technology has always been limited by its slow charging time and degradation of performance after a certain number of charge cycles. High energy density capacitors overcome the drawbacks of standard liquid electrolyte batteries as they exhibit charging times measured in minutes and a minimal decrease in performance over millions of cycles. This paper presents a new class of dielectric materials with relative permitivity on the order of several millions (5-6 $x10^6$) along with dielectric loss of <6% and temperature coefficient of capacitance of <12%. There many potential applications for this materials and devices and include single and multilayer capacitors in micro electronics, automotive, aerospace, heavy machinery, micro grid storage and large grid storage. In automotive industry, this technology will lead to the reduction of the out-of-service hours that current electric cars require to recharge, one of the largest consumer barriers for widespread market penetration.

G9: Innovative Processing of Metal Oxide Nanostructures, Heterostructures and Composite Materials for Energy Storage and Production

Innovative Processing

Room: York B

Session Chair: Thomas Fischer, University of Cologne

1:30 PM

(GFMAT-211-2019) Synthesis and Properties of Low-dimensional Titania Nanotube/Polyaniline Nanohybrids by In-situ Photo-polymerization (Invited)

K. Tsukatani[1]; S. Tsukuda[2]; T. Goto[1]; S. Chou[1]; T. Sekino*[1]

1. Osaka University, The Institute of Scientific and Industrial Research, Japan
2. Tohoku University, Institute of Multidisciplinary Research for Advanced Materials, Japan

Titania nanotube (TNT) has uique low-dimensional nanostructured materials which can be synthesized from TiO_2 powder by chemical processing. It is expected as energy production and environmental purification material because of its excellent photochemical properties, However, TNT only responsibles to ultraviolet (UV) light and has low electrical conductivity, To overcome these disadvantages, we are focusing on nano-hybridizing conductive polymer, here we choose polyaniline (PANI). In addition, we propose the new synthesis method of nano-hybridizing TNTs with PANI by photopolymerization without using any polymerization initiator. In this method, polyaniline is polymerized by radical species generated from TNTs by the incident UV light irradiation. Formation of polyaniline was confiemed by the UV light irradiation to the acidic aqueous solutions containing TNT and aniline monomer at 25 °C for 6h. When the pH was low, conductive polyaniline was formed and aggregated on TNTs. To synthesis more homogeneous immobilization of PANI to TNTs, linker molecules were immobilized to TNT surface, which could also act as linking molecule to PANI formation, Visible light responsible photocatalytic properties were confirmed for the TNT/PANI nanohybrids. Detailed synthesis processes, nano-hybrid structures and properties will be discussed.

2:00 PM

(GFMAT-212-2019) Oxide Bilayers as High Efficiency Water Oxidation Catalysts through Electronically Coupled Phase Boundaries (Invited)

T. Fischer*[1]; J. Leduc[1]; Y. Gönüllü[1]; S. Mathur[1]

1. University of Cologne, Institute of Inorganic Chemistry, Germany

New semiconductor metal oxides capable of driving water-splitting reactions by solar irradiation alone are required for sustainable hydrogen production. Whereas most metal oxides only marginally deliver the photochemical energy to split water molecules, uranium oxides are efficient photoelectrocatalysts due to their absorption properties (E_g ~ 2.0 - 2.6 eV) and easy valence switching among uranium centers that additionally augment the photocatalytic efficiency. Although considered a scarce resource, the abundance of uranium compounds in the environment is manifested in the huge quantities of stored UF_6 gas, produced as waste streams in the nuclear fuel enrichment process. Here we demonstrate that thin films of depleted uranium oxide (U_3O_8) and their bilayers with hematite (a-Fe_2O_3) are high activity water oxidation catalysts due to electronically coupled phase boundaries. The electronic structure of uranium oxides showed an optimal band edge alignment in U_3O_8//Fe_2O_3 bilayers (DFT calculations) resulting in improved charge-transfer at the heterojunction as supported by TAS and XAS measurements. The enhanced photocurrent density of the heterostructures with respect to well-known hematite offers unexplored potential of uranium oxide in artificial photosynthesis.

2:30 PM

(GFMAT-213-2019) Low-temperature Sintering Process of Bioactive Glass Nanoparticles Under Hydrothermal Conditions

Y. Seo*[1]; T. Goto[1]; S. Chou[1]; T. Sekino[1]

1. Osaka University, The Institute of Scientific and Industrial Research, Japan

Bioactive glasses are promising materials that have been investigated for various applications such as drug delivery and implant coatings. In general, to apply them for the scaffolds as well as other bulk applications, high-temperature sintering process is necessary. Recently, Cold Sintering Process (CSP), a densification process of ceramic materials at low temperature below 300 °C under a uniaxial pressure and aqueous solutions, was reported and its conditions are similar to hydrothermal conditions. Under the hydrothermal conditions, calcium-phosphate phases such as hydroxyapatite can be formed by biomineralization of bioactive glasses at their surfaces. In this research, we report the low temperature sintering process of bioactive glass nanoparticles through CSP coupled with biomineralization. First of all, SiO_2-CaO-P_2O_5 bioactive glass nanoparticles were synthesized by the sol-gel process using inorganic precursors. The obtained glass nanoparticles with aqueous solutions such as pure water and simulated body fluid solution were put into the mold and sintered under several hundred MPa from room-temperature to 200 °C to encourage the biomineralization at the interface between the glass nanoparticles. The formation of the glass nanoparticles, sintering process, densification behavior, and properties of the sintered bioactive glass nanoparticles will be discussed.

2:50 PM

(GFMAT-214-2019) The inhibition of hydrogen and oxygen recombination and over-all water splitting over Pt-TiO_2

G. Lu*[1]

1. Lanzhou Institute of Chemical Physics, China

Semiconductor photocatalysts for overall water splitting into H_2 and O_2 require metal cocatalyst, such as Pt, to catalyze H_2 evolution efficiently. However, these metal cocatalysts can also catalyze hydrogen and oxygen recombination to form water. In this work, we found that the pre-adsorbed halogen atom catalyst could inhibit the reverse reaction of water formation from H_2 and O_2 due to the decrease of adsorption energies of H_2 and O_2 on Pt. The adsorption energy decrease of H_2 and O_2 followed the order of F/Pt < Cl/Pt < I/Pt < Br/Pt. H_2-TPD results exhibited similar dependence. This inhibition was achieved via the occupation of halogen atom on the Pt surface sites, and thereby the adsorption and activation of hydrogen and oxygen molecules were decreased. The occupation difference of halogen atoms are determined by radius of halogen ions, which further leads the different activity for H_2 and O_2 recombination. By inhibition of water formation reverse reaction, the over-all water splitting over Pt/TiO_2 photocatalysts has been achieved. Isotope experiments with D_2O and $H_2{}^{18}O$ confirmed the over-all water splitting to H_2 and O_2. This study may help scientist to develop high-efficient photocatalyst for overall water splitting.

3:30 PM

(GFMAT-215-2019) Solution processing of complex nano-structured sponges (Invited)

G. Westin*[1]

1. Uppsala University, Sweden

Typical features required for materials to be used in sensors, catalysts, solar-cells and energy storage are a large interface to the surrounding liquid or gas phase and surface modification for e.g. catalysis, band structure and corrosion control. Typically, a high conductivity is required to get generated electrons in or out of the surface for electro-catalysts, sensors, solar cells and batteries, which is achieved by sponge structures of high crystalline quality and good connectivity though the structure. Here we present salt-based synthesis routes yielding oxide sponges of various contents at temperatures from 200 °C, 3 min. Systems such as doped and non-doped ZnO and MgO are discussed in detail from the solution to the final products, along with some properties. The sponges obtained at 200 °C typically consist of highly porous bread-like structures built from well-connected ca 10 nm crystallites. These sponges do not sinter together, even on heating to 900°C, but from ca 500°C, a reproducible grain growth took place within the sponge structures allowing for tuning of crystal sizes, in some cases up to 100+ nm. The processes and products were studied with; TG/DT/DSC, XRD, SEM-EDS, TEM-EDS/ED, XPS, IR- and Raman spectroscopy.

4:00 PM

(GFMAT-216-2019) Correlation between electron density of $SrTiO_{3-\delta}$ powder and hydrogen/oxygen evolution photocatalytic activities

S. Nishioka*[1]; J. Hyodo[2]; J. J. Vequizo[3]; S. Yamashita[4]; H. Kumagai[1]; K. Kimoto[4]; A. Yamakata[3]; Y. Yamazaki[2]; K. Maeda[1]

1. Tokyo Institute of Technology, Japan
2. Kyushu University, Japan
3. Toyota Technical Institute, Japan
4. National Institute for Materials Science (NIMS), Japan

Metal oxides have been widely studied as photocatalytic water-splitting materials because of their high stability in water under irradiation. Defects in semiconductor photocatalysts have a significant negative impact on photocatalytic activity for overall water splitting reaction. Some recent reports clearly showed enhancement of photocatalytic activity for the half reactions of hydrogen or oxygen evolution by the introduction of defects. However, no quantitative correlation between the defects and photocatalytic activity has been obtained in any of reported powder-based semiconductors to date. To understand the quantitative correlation, we have focused on the electron density, which increases with the density of oxygen vacancies due to charge compensation of the system. In this study, the non-stoichiometry of $SrTiO_{3-\delta}$ powder was precisely controlled by annealing oxygen partial pressure without changing other physicochemical properties. The photocatalytic activities of $SrTiO_{3-\delta}$ for hydrogen and oxygen evolution were enhanced respectively forty-fold and three-fold with an increase in the electron density. Electron doping shifted the Fermi level toward negative and expanded the degree of surface band bending. The improvements of photocatalytic activities correlated well with these two factors generated the electron doping.

4:20 PM

(GFMAT-217-2019) Preparation of thin film in low-dimensional spin system toward electric control of thermal conductivity

N. Terakado*[1]; Y. Machida[1]; Y. Nara[1]; S. Watanabe[1]; Y. Takahashi[1]; T. Fujiwara[1]

1. Tohoku University, Japan

We aim to fabricate materials and devices possessing electrically controllable thermal conductivity which contribute effective heat dissipation and high stability in the electronic devices and accordingly we have focused on spin thermal conductivity materials, e.g., La–Ca–Cu–O (LCCO). In the materials, S=1/2 spins of Cu^{2+} which are antiferromagnetically coupled by O^{2-} are heat carrier, so that the materials show high, anisotropic thermal conductivity even at room temperature. We expect that the thermal conductivity can be controlled by electrically/electrochemically induced structure change. In this report, we fabricated spin thermal conductivity films and multilayers with SiO_2, which were sandwiched by electrodes. For the LCCO films, we investigated structure and thermal properties under application of an electric field by Raman spectroscopy and frequency-domain thermoreflectance method. We discuss change in structure and thermal properties on the basis of the results and additionally scanning transmittance microscopy and element mapping. In addition, we will show orientation control for improvement in thermal conductivity.

4:40 PM

(GFMAT-218-2019) Novel Tetra-cation Organometallic Halide-based Perovskite Solar Cell

P. Dey[1]; T. Maiti*[1]

1. Indian Institute of Technology Kanpur, Materials Science and Engineering, India

The research works on methylammonium lead iodide ($CH_3NH_3PbI_3$) based perovskite solar cell (PSC) skyrocketed over the past couple of years, making it one of the break-through materials of this decade. However, there are some serious issues like the toxicity of lead, poor durability in hot and humid conditions which are needed to be addressed for the commercialization. Here, we showed that designing triple-cation B-site in $CH_3NH_3PbI_3$ perovskite by introducing bismuth (Bi) in combination with Na/K at Pb-site can improve the stability of PSC w.r.t moisture and heat. We also studied formamidinium ($H_2NCHNH_2^+$) based tetra-cation PSC. Large crystals with compact microstructure were found in FESEM. Moreover, the EDS in conjugation with XPS analysis confirmed the compositional homogeneity. UV-Vis spectra demonstrated a high absorption coefficient in the visible spectrum with an optical band gap in the range 1.7-1.9 eV. Fluorescence decay kinetics measurement exhibited a carrier lifetime on the order of a nanosecond. We obtained PCE ~0.5% in the planar PSC based on these compositions. TGA-DSC measurement confirmed temperature stability up to 240°C for these materials. We studied XRD patterns as well as UV-Vis spectra for 15 days period, illustrating no sign of degradation. Furthermore, femtosecond transient absorption spectroscopy was carried out to understand the charge recombination process in these perovskites.

G11: Smart Processing and Production Root Technology for Hybrid Materials

Smart Processing for Hybrid Materials

Room: Salon C
Session Chair: Tadachika Nakayama, Nagaoka University of Technology

1:30 PM

(GFMAT-219-2019) Oxide glass-ceramics for all-solid state Na ion batteries (Invited)

T. Honma*[1]; T. Komatsu[2]

1. Nagaoka Univeristy of Technology, Department of Materials Science and Technology, Japan
2. Nagaoka University of Technology, Japan

In recent years, applications of Lithium ion batteries have been considered from energy storage devices of mobile-type equipment such as laptop to large energy storage devices such as electric vehicle. Increasing demand for Li chemicals combined with the limited Li mineral reserves will drive up prices. Based on the wide availability and low cost of sodium, sodium ion batteries(NaB) have the potential for meeting large scale energy storage. We successfully synthesized $Na_2FeP_2O_7$ (NFP) glass-ceramics through the crystallization of stoichiometric $Na_2FeP_2O_7$ glass powders and proposed that those glass-ceramics have a potential of the safety cathode candidate for NaBs with low materials cost. In addition, the demonstration of the driving all-solid state sodium ion batteries composed of NFP and β″-alumina solid electrolyte have been done at room temperature. The most of advantage why we use glass and glass-ceramics to develop all-solid state batteries is as follows; (1)glass exhibits softening above glass-transition temperature, (2)it is easy to join between active materials and solid electrolyte. In this study, we discuss the crystallization behavior of NFP and the other phosphate glasses that useful for NaBs.

2:00 PM

(GFMAT-220-2019) Effects of Adhesives Types on Interfacial Strength Evaluation Method for Plasma-Sprayed Hydroxyapatite Coating (Invited)

Y. Otsuka*[1]

1. Nagaoka University of Technology, System Safety, Japan

The purpose of this study is to evaluate interfacial strength of plasma-sprayed HAp coating by using more general adhesives. Plasma-sprayed HAp coating has been applied to bond bones with the surfaces of artificial hip joints. However, HAp coating is subjected to crack or delamination by mechanical loading. Conventional standard codes for measurement of interfacial strength of calcium phosphate coating determine the use of a specific adhesive irrationally. Our group previously proposed preimmersion treatment process in preparation of interfacial testing specimens in order to obtain valid value of interfacial strength. However, the type of the adhesive was for medical purpose and not general one. To widen applicability of the proposed method, a selection policy of adhesive is indispensable. Metal Lock Y610 (ML adhesive) was selected as one of general adhesives. Interfacial strength tests by using ML adhesive were conducted. The results of interfacial strength test were compatible with the one reported by previous study, which suggest that the selection of general type of adhesive was successful. Raman spectroscopy analyses were also conducted to confirm a suppressed infiltration of ML adhesives.

2:30 PM

(GFMAT-221-2019) Pyroelectric power generation with 7mol% La-modified Lead Zirconate Titanate PLZT (7/65/35)

K. B. Parussangi*[1]

1. Nagaoka University of Technology, Department of Mechanical Engineering, Japan

The combination of novel electrothermodynamic cycle based on temporal temperature variations and the pyroelectric effect is one of the potential method for utilizing the waste heat energy as a renewable energy source. Lanthanum-modified lead zirconate titanate (PLZT) ceramics with concentration of La (5-7%), are located at and near the phase boundary between the rhombohedral and tetragonal ferroelectric phases at room temperature, which shows that these ceramics are possible as the candidates for a further improvement of power generating performance. In this study, we propose the relaxor ferroelectric ceramic 7mol% La-modified Lead Zirconate Titanate PLZT (7/65/35), which is known for its high density, squareness of hysteresis loop and high dielectric constant. The power generating potential is evaluated theoretically by using hysteresis loop and pyroelectric coefficient measurement, and experimentally by using the DSW circuit to convert waste heat to practical energy.

2:50 PM

(GFMAT-222-2019) A C-S-H Builder and Interface Modeling Tools towards Accurate Reactive Full Electrolyte Simulations of Cement Materials up to the Micrometer Scale

D. Guittet[2]; T. Jamil[2]; H. Heinz*[1]

1. University of Colorado-Boulder, USA
2. University of Colorado, Department of Chemical and Biological Engineering, USA

Cement and concrete are prime building materials with superior properties, however, they continue to cause high CO_2 emissions. One of the ways to modify these drawbacks is better understanding of the underlying hydration and setting reactions, and introduce alternative minerals with lower carbon footprint. Specifically, calcium-silicate-hydrates (C-S-H) are the major hydration products and their role has not yet been well understood. We introduce a GUI-based automated C-S-H model builder across a range of C/S and C/H ratios, as well as new models for aluminate and oxide additives in cement that can be used with the Interface force field and multiscale simulation programs to understand the hydration and setting process from the atomic scale to the micrometer scale (NAMD, GROMACS, LAMMPS, Materials Studio). We discuss the validation of models and first applications to elucidate the role of PCE polymers and carbohydrates in cement hydration in comparison with measurements. The inclusion of ionic strength, pH, and metadynamics for sampling is described. The quality of structures, surface, and hydration energies as well as mechanical properties exceeds the reliability as DFT methods at lower computational cost, and we epxlain how chemically detailed simulations can be extended for macroscale property predictions.

3:30 PM

(GFMAT-223-2019) Evaluation of Mechanical Property by Micro Slurry-Jet Erosion Test in Ceramics (Invited)

Y. Miyashita*[1]; Y. Kihara[1]; T. Katsumata[2]; T. Matsubara[2]

1. Nagaoka University of Technology, Department of Mechanical Engineering, Japan
2. Palmeso Corporation Limited, Japan

Micro slurry-jet erosion test has been developed as a new testing method to evaluate material property. In the test, slurry is applied to surface of material evaluated and erosion rate is measured. This testing method does not completely destroy materials but the damage induced is microscopically local. It is speculated that information of materials such as microstructure and mechanical properties are included in the testing result of micro slurry-jet erosion test because scale of erosion occurred is comparable with microstructural scale. However, its mechanism is not clearly understood yet. In the present study, relationship between mechanical property and the erosion behavior was investigated. Alumina ceramic with fine grain size was produced by spark plasma sintering. Heat treatment was then applied to obtain different grain size. Results of micro slurry-jet erosion test showed that different erosion rate was observed in alumina with deferent grain size. Fracture toughness, bending strength and hardness were measured as mechanical properties. Relationship between mechanical properties and erosion rate due to change in grain size was discussed with consideration of erosion mechanism in the testing method.

4:00 PM

(GFMAT-224-2019) Self-healing properties of die-silicate compound-based composite material (Invited)

T. Nakayama*[1]

1. Nagaoka Univ of Tech, Japan

This work evaluates the effect of TiC addition on $Y_2Ti_2O_7$-Y_2TiO_5 (YT75) ceramics on their mechanical properties and promotion of a self-healing process. Several $Y_2Ti_2O_7$-Y_2TiO_5-TiC composites (YT75C) were fabricated by using solid state reaction and hot-press sintering at 1500°C for 1 h in Ar at 25 MPa. All YT75C composites were annealed at 1200°C in air for 6 h to promote the oxidation of TiC into TiO_2, and then, induce a chemical reaction between Y_2TiO_5 and TiO_2 to form new $Y_2Ti_2O_7$ phase, evidencing a self-healing process. X-ray diffraction (XRD) was used to characterize the phase transformations before and after annealing, whereas scanning electron microscope (SEM) was used for observing TiC distribution on the YT75C surface. Vickers hardness and fracture toughness of YT75 and YT75C composites were evaluated at different TiC additions. Results confirmed the promotion of a self-healing process in YT75C composites after annealing. It is expected that an adequate amount of TiC addition could enhance the mechanical properties of YT75 ceramics and promote a self-healing process in YT75C composites, simultaneously.

4:30 PM

(GFMAT-225-2019) Adsorption of Pb and Cd in rice husk and their immobilization in glass-ceramic structure

E. Sharifikolouei*[1]; F. Baino[1]; M. Salvo[1]; D. Fino[1]; M. Ferraris[1]

1. Politecnico di Torino, Department of Applied Science and Technology, Italy

Rice husk (RH), an agricultural waste, is abundantly available in many countries such as China, India, Brazil, US, and South East Asia. Despite the massive production of rice husk, it is mainly disposed to landfill. In this work, rice husk was first used as an adsorbent to adsorb Pb and Cd from waste-water and then was incorporated inside a glass structure to immobilize the heavy metals and was further used to be incorporated inside a porous glass-ceramics structure. The final glass-ceramic could be implemented as insulating materials in the construction industry. For this purpose, first, 3 batches of glasses were prepared from different ratios of recycled glass and foaming agents (40:60, 50:50, 60:40). It was shown that the 40:60 ratio generates the optimum porosity distributions within the glass. Rice husk, containing heavy metals, was then added to this glass and was heat treated for 3h at 750° C. The leaching test on the final glass-ceramic confirmed the immobilization of heavy metals. The mechanical test was also performed to investigate the practical use of this glass-ceramics for insulating applications.

4:50 PM

(GFMAT-226-2019) Development of mixing method of ceramics powder using electric field

T. Nakayama*[1]

1. Nagaoka Univ of Tech, Japan

Conventionally, mixing of ceramics was often performed by mechanical mixing method. However, in these methods, problems of contamination have been pointed out. In addition, maintenance problems such as sticking to containers are pointed out. On the other hand, it is known that materials can be stirred by using an electric field. In this paper, the powder was agitated in a solvent while applying a large electric field without dielectric breakdown by using nanosecond pulsed electric field. In this method, the conventional mechanical mixing method

5:10 PM

(GFMAT-227-2019) Investigation of pyroelectric power generation amount by controlling Sn:Ti ratio of PLZST

H. Sugiyama*[1]; Y. Kawamura[1]; K. B. Parussangi[1]; N. Ishibashi[1]; H. Yoshimura[1]; M. Takeda[1]; N. Yamada[1]; H. Hashimoto[2]; T. Goto[2]; T. Sekino[2]; T. Nakayama[1]

1. Nagaoka Univ of Tech, Japan
2. Osaka University, The Institute of Scientific and Industrial Research, Japan

In power regeneration from a heat source with temporal temperature change (dT/dt), the research is being carried out focusing on pyroelectric effect of ferroelectric. The new thermal/electric combined cycle that applies external charge according to the temporal temperature change is expected to further increase the amount of power generation compared with the conventional cycle. However, there are few experimental examples. In this study, La-doped Pb(Zr, Sn, Ti)O3 (PLZST) ceramics was applied as a pyroelectric material, and power generation characteristics and electric characteristics were measured. PLZST becomes paraelectric phase (PE) after passing through ferroelectric rhombohedral (FER), antiferroelectric tetragonal (AFET) with increasing temperature. In addition, the phase transition from FE to AFE is promising as a pyroelectric sensor material. The phase transition threshold and electric characteristics were adjusted by controlling the Sn:Ti ratio of PLZST. In addition, the power generation amount at that time was compared. As a result, it was found that electric power can be regenerated over a wider temperature range by controlling Sn:Ti ratio.

G15: Advanced Luminescent Materials and Their Applications

Luminescent Materials and Applications

Room: Salon D

Session Chairs: Rong-Jun Xie, Xiamen University; Jianhua Hao, Hong Kong Polytechnic University

1:30 PM

(GFMAT-228-2019) Novel Approaches for Stabilizing Luminescent Lead Halide Perovskite Materials and Their Applications in Analytical Sensing (Invited)

F. M. Li[1]; H. Z. Kang[1]; Y. Jiang[1]; X. Chen*[1]

1. Xiamen University, China

Pervoskite nanocrystals (PNCs) have been received a lot of attention nowadays, due to their exceptionally high photoluminescence quantum yields and tunability of their optical band gap over the entire visible spectral range by modifying composition or dimensionality/size. Benefits from these outstanding characteristic, PNCs have demonstrated promising applications in LEDs, laser, and photocatalysts et al. But their application in analytical chemistry is still remains a big challenge since their poor reproducibility of synthesis and stability. In this topic, my group recent works on PNCs will be introduced including a new aliphatic nucleophilic substitution guided synthesis of PNCs as well as a hollow SiO_2 template guided onsite fabricating PNCs. As the old saying goes: every cloud has a silver lining. The sensitive nature of PNCs in fact provides an opportunity to turn this drawback into an advantage in analytical sensing including O_2, humidity, temperature and halide ions et al.

2:00 PM

(GFMAT-229-2019) Synthesis and Fluorochromic Properties of Eu^{3+}-activated Tungstate Phosphors

S. Fujihara*[1]; H. Ye[1]; R. Hara[1]; M. Hagiwara[1]

1. Keio University, Japan

Fluorochromism is a phenomenon where fluorescence or luminescence is changed in response to external physical or chemical environment. We have attempted to induce fluorochromism in metal tungstate phosphor materials such as $CaWO_4$:Eu^{3+} and Y_2WO_6:Eu^{3+}. First, powders of $CaWO_4$:Eu^{3+} and Y_2WO_6:Eu^{3+} were synthesized by a hydrothermal reaction method. The structure of individual particles in the resultant powders was characterized as micrometer-sized aggregated particles (microspheres) consisting of primary nanoparticles. The $CaWO_4$:Eu^{3+} and the Y_2WO_6:Eu^{3+} powders exhibited good fluorochromic properties in response to reductants and oxidants in liquid and gas media, respectively, due to their high specific surface area. We also synthesized platinum-loaded Y_2WO_6:Eu^{3+} powders through the liquid-phase deposition of Pt nanoparticles using a $PtCl_6^{2-}$ solution. The redox response of the Pt/Y_2WO_6:Eu^{3+} powders was then enhanced by a catalytic effect of platinum. Thin films of Y_2WO_6:Eu^{3+} were also synthesized, aiming at a facile monitoring of hydrogen gas by luminescence switching. It was shown that a porous Y_2WO_6:Eu^{3+} thin film was superior to a dense one in terms of the redox sensitivity. All the above results demonstrate that the fluorochromism is promising as a new mechanism of chemical sensing of redox species.

2:20 PM

(GFMAT-231-2019) Luminescent Materials for Laser-Driven Solid State Lighting (Invited)

R. Xie*[1]; L. Wang[2]

1. Xiamen University, China
2. China Jiliang University, China

Laser-driven solid state lighting is superior to white light-emitting diodes (wLEDs) in terms of super-high brightness, long lighting distance, small volume and high luminous efficacy, which is now attracting increasing attentions. Differring from those materials used in wLEDs, luminescent materials for laser-driven solid state lighting must bear much higher blue laser irradiation densities, which therefore should have small thermal quenching, high ability of thermal dissipation and high quantum efficiency. In this presentation, we will report several types of luminescent materials for laser-driven solid stata lighting, including phosphor ceramics, phosphor-in-glass bluks, and phosphor-in-glass films. The luminance saturation of luminescent materials will be discussed. Finally, we demonstrate laser-driven white light by using these interesting luminescent materials.

3:30 PM

(GFMAT-232-2019) The f-d transitions of Ce^{3+}, Pr^{3+} and Eu^{2+} in silicates for potential display and detecting applications (Invited)

H. Liang*[1]

1. Sun Yat-sen University, School of Chemistry, China

Nowadays, much attention is being addressed to f-d transitions of lanthanide ions in different hosts for applications in lighting and displays. As important host compounds of luminescence of lanthanide or transition metal ions, silicates have attracted much attention due to their good chemical and thermal stabilities. Ce^{3+}, Pr^{3+} and Eu^{2+} are typical rare earth ions with parity allowed f-d transitions in most silicates. They usually exhibit broad emission bands with short decay times, thus Ce^{3+}, Pr^{3+} and Eu^{2+} doped materials have potential applications as phosphors and scintillators. Herein, we report our recent work on luminescence of Ce^{3+}, Pr^{3+} and Eu^{2+} in silicates $Sr_{(8-x)}Eu_x(Si_4O_{12})Cl_8$, $Ba_2MgSi_2O_7$, $BaMg_2Si_2O_7$, $LiYSiO_4$ and $BaY_2Si_3O_{10}$.

4:00 PM

(GFMAT-233-2019) Luminescent 2D layered semiconductor nanosheets doped with lanthanide activated ions (Invited)

J. Hao*[1]

1. Hong Kong Polytechnic University, Hong Kong

Lanthanide ion activated luminescent materials have been widely used in optoelectronic devices and biomedicine. In particular, lanthanide ions that can emit near-infrared (NIR) photons have been widely studied. On the other hand, as the size of the devices is progressively approaching the limits of conventional semiconductor technology. Owing to their atomic scale thickness, 2D layered semiconductors have attracted a great deal of interest. Here, my group has first introduced lanthanide dopants into 2D layered hosts and realize NIR-to-NIR down- and up-conversion photoluminescence. The deposition conditions are precisely controlled to obtain thin films (e.g., MoS_2: Er and WSe_2/Yb/Er) with the desired layer number. The crystal structure and chemical composition of the films were determined. Importantly, the luminescence of 2D materials simply pumped by a single NIR laser diode can be extended to a wide range of NIR spectrum, including telecommunication range at 1.55 μm, which can expand the intrinsic narrow-band emission of 2D layered semiconductors. The works open a door to greatly extend the luminescence wavelengths of 2D semiconductors, which will benefit for not only investigating fundamental issues, but also developing atomically thin devices. The works are supported by the grant from Hong Kong RGC GRF (PolyU 153281/16P).

4:30 PM

(GFMAT-234-2019) Scandium-Based Luminescent Nanomaterials (Invited)

L. Huang*[1]

1. Nanjing Tech University, China

In the past decades, rare earth-based photon upconversion luminescent nanomaterials have drawn greatly increased attention due to their superior optical properties. However, majority of the attention has been focused on Y- and lanthanide-based nanomaterials while there is very few reports on Scandium-based nanomaterials although Sc sits at a very unique position in the periodic table, i.e., the cross junction between the top of the rare earth column and the beginning of the transition metal row. Herein, we will summarize our recent advances on the chemistry of Sc-based nanomaterials, their luminescent properties, as well as potential applications, which indeed show the uniqueness of Sc comparted to other rare earth elements.

5:00 PM

(GFMAT-235-2019) Ab Initio molecular dynamics study of structure-composition-property relationships in phosphors

M. Amachraa*[1]; H. Tang[1]; C. Chen[3]; Z. Wang[2]; S. Ong[3]

1. University of California, San Diego, Materials Science, USA
2. Technical University of Denmark, Physics, Denmark
3. University of California, San Diego, Department of NanoEngineering, USA

Phosphor-converted white light-emitting diodes (pc-WLEDs) have been widely adopted for next-generation solid-state lighting mainly. However, our understanding of thermal-quenching (TQ), i.e., the loss in PL intensity with temperatures, remains incomplete, with several competing theories. In this work, we demonstrate the application of ab initio molecular dynamics (AIMD) simulations as a novel approach to investigate the effect of temperature on Eu^{2+}/Ce^{3+} local environment. A statistical analysis of the activator local environment is extracted from the atomic trajectories from AIMD at multiple temperatures revealing a clear relationship between the temperature-dependent activator local environment, and the experimentally-measured TQ in numerous well-known phosphor compounds. We have found that phosphors with low TQ show a small variability in their activator's local environment distribution within the operating temperature range. We propose a model where the activator local environment fluctuations due to temperature lead to changes in the crystal field splitting around the activator, which in turn have a consequence on the photoionization barrier and TQ behavior. Finally, we propose structural descriptors based on these observations that can be used to rapidly screen novel materials for high quantum efficiency phosphors with excellent TQ resistance.

Young Professionals Forum - Next Generation Materials for Multifunctional Applications and Sustainable Development, and Concurrent Societal Challenges in the New Millennium

Advances in Biomedical Science and Engineering III

Room: York A

Session Chair: Eva Hemmer, University of Ottawa

11:30 AM

(YPF-020-2019) Translational Biomaterials: How interdisciplinary Science can be put to work (Invited)

E. I. Alarcon*[1]

1. University of Ottawa, Biochemistry, Microbiology and Immunology, Canada

The current body of literature supports the need for developing novel materials for clinical uses. Numerous are the steps needed to expedite the safe clinical translation of materials. In the present talk, we will discuss how the development of biomaterials can be optimised for safe clinical translation while keeping discovery and innovation at the core of the process for corneal and cardiac tissue repairs.

Friday, July 26, 2019

G4: Porous Ceramics for Advanced Applications through Innovative Processing

Porous Bioceramics II

Room: Trinity III

Session Chair: Alberto Ortona, SUPSI

8:30 AM

(GFMAT-237-2019) Osteoconductive microarchitecture of ceramics realized by additive manufacturing for bone tissue engineering (Invited)

F. E. Weber*[1]

1. University Zurich, Center for Medical Dentistry/Oral Biotechnology & Bioengineering, Switzerland

If a porous bone substitute scaffold is placed in a bony defect, the bone starts to grow into this microarchitecture. This phenomenon is called osteoconduction. The aim of this project is to determine the most osteoconductive microarchitecture in a ceramic scaffold, which accelerates and enhances bone ingrowth and avoids the formation of non–unions, the worst clinical outcome of a bone fracture. A library of diverse microarchitectures was designed and produced via lithography in a layer-by–layer approach from tri-calcium phosphate or bioglass. The biological testing of these scaffolds was performed in calvarial bone defects. The histomorphometric analysis, based solely on the middle section, revealed that bone formation was significantly increased in all implant treated groups. The microarchitecture with the highest osteoconductivity was characterized by pores of 1.2 mm in diameter. In conclusion, optimal osteoconductive porous lightweight structures from ceramics have potential for bone regeneration and augmentation purposes, especially when complex microarchitectures and patient-specific geometries are essential. Therefore, additive manufacturing will be a key component in the realization of personalized bone regeneration procedures; where for each patient a specific scaffold is produced to treat bone defects in orthopedics, cranio-maxillofacial surgery and dentistry.

9:00 AM

(GFMAT-238-2019) Additive manufacturing of ceramic-based materials for bioapplications: A state of the art of the activity in the field at the Institute of Research for Ceramics (IRCER, Limoges, France) (Invited)

F. Rossignol*[1]

1. Institute of Research for Ceramics (IRCER), UMR CNRS 7315, France

We will give here an overview of what is being done in the field of Additive Manufacturing (AM) at the Institute of Research for Ceramics (IRCER) located in Limoges, France. IRCER is the largest academic institution in its field in Europe and has been working on AM technologies for the last 20 years. Here, we will show recent progresses linked to the fabrication of implants for bone tissue engineering and of advanced biosensors. We will also discuss about the future challenges of AM of ceramic-based materials.

9:30 AM

(GFMAT-239-2019) 3DP of bioceramics with accurate hierarchical pores for personalized maxillofacial repair

C. Zhou*[1]; B. Zhang[1]; Y. Fan[1]; X. Zhang[1]

1. Sichuan University, China

Hierarchical porosity, which includes micropores and macropores in scaffolds, contributes to important multiple biological functions for tissue regeneration. However, most of these conventional methods are difficult to control the scaffolds' pore arrangements and dimensions. Concerning the biological function importance of hierarchical macro-/micro-porosity, this study seeks to construct hierarchical porous HA bone tissue engineering scaffolds with rigid porous structures using 3DP. HA with nano-sized crystals of 30–50 nm with lengths of 50–100 nm were modulated by polyvinyl alcohol, cellulose, and pure water to form the printing "ink". The first-level macropores of HA scaffolds were designed by CAD molding with considering of 20% linear shrinkage, and fabricated by the 3DP technique. The second-level micropores of scaffolds were obtained by the freeze and sintering process. Results showed the hierarchical microstructure of 3DP bioceramics have highly open, well-interconnected, and uniform pores. The bioceramics with precise porosity showed obvious osteoinductivity in the animal experiments. This research may provide a versatile way to modulate biological function of biomaterials through optimized design and fabrication of scaffolds.

Processing and Engineering Applications of Porous Ceramics

Room: Trinity III

Session Chairs: Franz Weber, University Zurich; Fabrice Rossignol, Institute of Research for Ceramics (IRCER)

10:10 AM

(GFMAT-240-2019) Cellular ceramics produced by additive manufacturing and coated with natural zeolite: A new class of filter for the adsorption of micro-pollutants in waste and surface waters (Invited)

R. Koenig[1]; G. Bianchi[1]; M. Spaggiari[1]; A. Ortona*[1]

1. SUPSI, MEMTi, Switzerland

A filter made of engineered cellular ceramics and coated with natural zeolite was produced to address the increasing issue of filtering new contaminants into water reservoirs. Increasing use of drugs and the implementation of finer analytic tools has created an new awareness of waste substances into drinking water. Micro-pollutants are present in minimum concentrations within our environment. Sources of the pollutants are the municipal wastewater treatment plant effluents, where substances such as: antibiotics, anti-inflammatory drugs, corrosion inhibiters or antidepressants are accumulating into the environment. We developed a filter prototype able to adsorb micro-pollutants. The filter support is made of 3D printed alumina and dip coated with natural zeolite. Its architecture is optimized according to its final use. Adsorption efficiencies of twelve target substances (industrial and pharmaceutical compounds) showed an elimination capacity from 40% up to 80% if surface modified zeolite was adopted. Today's state of the art technologies, ozone treatment and adsorption on activated carbons are well established, but present some drawback. Engineered alumina/zeolite filters, able to regenerate and easy to apply, will move water filtration toward a more efficient and sustainable process.

10:40 AM

(GFMAT-241-2019) Pseudoboehmite–polymethylsilsesquioxane macroporous monoliths formed by colloidal gelation

G. Hayase*[1]

1. Tohoku University, Japan

Colloidal dispersions of pseudoboehmite with various shapes and sizes, such as spherical particles, rods, fibers are commercially available. By coating and adhering the pseudoboehmite colloids with the trifunctional silicon alkoxide methyltrimethoxysilane via a simple sol-gel process, macroporous monoliths could be fabricated. In the case of using pseudoboehmite nanofibers, obtained monoliths had a characteristic fiber-like skeleton derived from the nanofibers. They exhibited relatively high mechanical strength and good thermal insulation properties. In this presentation, the formation mechanism of the monoliths having a core-shell structure and the physical properties when using various forms of colloids are discussed.

11:00 AM

(GFMAT-242-2019) Developing Porous Glass and Ceramic Microspheres for Water Treatment Applications

I. Ahmed*[1]; S. Samad[1]; E. Lester[1]

1. University of Nottingham, Faculty of Engineering, United Kingdom

Research scientists are currently focussing efforts on developing more sustainable material alternatives taking into consideration the environmental impact of material production. Novel materials are continually being sought to minimise/eliminate potential negative environmental impacts favouring their sustainability. Glasses, glass-ceramics and ceramics could be considered as suitable sustainable materials since they can be recycled, remade and reused over and again. In this project, we initially developed porous phosphate glass microspheres using a single-stage flame spheriodisation process and investigated their potential for removing micro-pollutants, using dye absorption tests. However. phosphate-based glasses would not be considered suitable for this application. We then exploited this processing route for recycled glass waste materials followed by naturally occurring magnetite. Initial trails have shown that formation of porous microspheres from both recycled glass waste and magnetite materials was successful. The magnetite materials have also undergone successful dye absorption tests (using acid red dye). This new manufacturing method has enabled processing of glass, glass-ceramic and ceramic materials into porous spherical structures with the potential for use in wastewater treatment applications.

11:20 AM

(GFMAT-243-2019) Manufacture of high porous SiC to be used as catalysis suport

J. Narciso*[1]; M. R. Caccia[1]; A. Ortega[1]

1. Alicante University, Spain

On catalysis there are two widely used catalyst supports, gamma alumina and zeolites. They are used for their high specific area, being inert in many media and can use without problems until an intermediate temperature. However, it does not meet the moost important requirements, such as high thermal conductivity. This is very important because it allows us to have a temperature control. So a possible candidate to be used is SiC, since it may have thermal conductivity higher than Cu, although it is usually not so high, since it is 220 W/mK, which is just double that of brass or 5 times higher than conventional steel. In addition its use will be extended to 1000 C without any problem. The great challenge that presents the SiC is its manufacture with an area greater than 100 m^2/g. What is the minimum area needed to can be used as catalyst support. SiC has an area of less than 1 m^2/g, and it has been reported in SiC beta literature with areas of about 27 m^2/g. In the present work a new method for the manufacture of SiC is presented where it is shown that it is It is possible to obtain SiC with an area greater than 100 m^2/g as well as not being microporous, which would make it difficult to Use as catalyst support. The idea is to synthesize a silica with an adequate pore distribution and subsequently perform CVD a deposit of a few layers of graphene in the pores that will allow us to obtain later the SiC.

11:40 AM

(GFMAT-244-2019) Argon microbubbles enhance strength and toughness in borosilicate glass

B. Wang*[1]

1. Xi'an Jiaotong Universitty, State Key Laboratory for Mechanical Behavior of Materials, China

An innovative processing route for developing porous borosilicate glass with argon microbubbles has been developed. The first stage of microcellular glass processing involves dissolving argon under high pressure (10~100 MPa) and high temperature (1373 K) into borosilicate glass to saturate it up to the equilibrium gas concentration, i.e., the solubility. Once a saturated glass is formed, a number of microvoids are rapidly nucleated by introducing a thermodynamic instability via pressure drop and heating. After annealing at softening temperature (1073 K) under low pressure (2.5~10 MPa), borosilicate glass with pressurized argon microbubbles could be obtained. The flexural strength and compressive strength of the porous glass with pressurized argon microbubbles was much high than that of similar porous glass, in which enclosed gas pressure was ~0.1 MPa. High bending strength of 71.6 MPa could be obtained for the H100A10 sample with enclosed gas pressure of ~15.7 MPa, which was higher than that of dense Pyrex glass of 69 MPa. Argon microbubbles implantation is shown to be an effective way to tune an internal length scale effect on strength.

G6: Multifunctional Coatings for Sustainable Energy and Environmental Applications

Aerosol Deposition Processes

Room: Trinity II
Session Chair: Rogerio Lima, National Research Council of Canada

8:30 AM

(GFMAT-245-2019) Highly Transparent Al_2O_3 Film and Deep Black Colored Al_2O_3 Film Fabricated by Using Aerosol Deposition Process (Invited)

J. Park*[1]; D. Kim[1]; H. Seok[1]; K. Lee[1]

1. IONES Co., Ltd., Republic of Korea

In recent, advanced surface treatment process in mobile cover glass has been developed with various coating technology. Especially, for anti-scratch and highly damage resistance, ceramic materials coating on mobile cover glass is in the limelight. Aerosol Deposition (AD) is used only kinetic energy of ceramic powder for coating. If ceramic powder size is reduced below 1um, ceramic powder is possible to plastic deforming on substrate by the local thermal energy generated from the impact energy. So, AD process is possible to coat on mobile glass at room temperature. Two type of ceramic coating, highly transparent Al_2O_3 film and deep black colored Al_2O_3 film was fabricated by using AD process. Transmittance of the transparent Al_2O_3 coating was about 90% at visible range and higher than the transmittance of sapphire glass. The crystal phase of sapphire is alpha alumina phase, and it was confirmed that the sapphire coating film is composed of several tens nanometers alpha-alumina grains by TEM. Hardness of the transparent Al_2O_3 coating is around1800 HV. It has been proved that the sapphire coating by aerosol deposition can contribute to the improvement of characteristics of mobile cover glass.

9:00 AM

(GFMAT-246-2019) Shadow-optical visualization of the gas jet formation in the Aerosol Deposition Method

P. Glosse*[1]; S. Denneler[2]; O. Stier[2]; D. Hanft[1]; R. Moos[1]

1. University of Bayreuth, Department of Functional Materials, Germany
2. Siemens AG, Germany

The aerosol deposition method (ADM) is a low-cost coating technology working at room temperature. An aerosol formed from a powder and a carrier gas is accelerated through a nozzle onto a substrate placed in a vacuum chamber. The collision of the powders particles with the substrate induces particle fracture and a fine-grained dense film forms. Magnesium diboride (MgB_2) is a promising superconducting material with high critical temperature of 39 K. Since MgB_2 exhibits ceramic-like brittle fracture properties, it is possible to produce films with the ADM from this material on substrate materials like glass and nickel base alloys. Parameters such as the gas volume flow and the vacuum chamber pressure strongly influence the film formation, which for example leads to a change in the film-thickness profile. A shadow optical setup was configured to visualize different density regions of the jet flow formation between the nozzle and the substrate. Shadow images were taken for various coating parameters without particle loading of the carrier gas. Films were also produced with the same sets of parameters, using a particle-loaded carrier gas. A correlation of the shadow images and the as-deposited film-thickness profiles hints to a model of the particle trajectories in front of the substrate.

9:20 AM

(GFMAT-247-2019) New coating method for optically down converting composite layers via aerosol deposition process (Invited)

S. Kim[2]; M. Cho[1]; S. Kim[2]; J. Oh*[1]

1. Kwangwoon University, Electronic materials engineering, Republic of Korea
2. Ajou University, Molecular Science and Technology, Republic of Korea

Distinct from conventional ceramic coating processes requiring thermal cost and complex process, the aerosol deposition (AD) process based on shocking loading solidification is a simple ceramic film preparation technique, featuring the high-speed direct coating of accelerated particles at room temperature. Moreover, the process can create ceramic-based composite films retaining intrinsic properties of raw materials. These many superior merits of the AD process have stimulated many researchers in different fields. Using the process, it has been actively studied for various applications including electronic/magnetic/optic devices, fuel cells, batteries, protective coatings, bio-component coatings, sensors, and so on. In this study, taking into the advantages of an AD process mentioned above, we developed a new coating method for the preparation of optically down converting composite films. This method can be employed in useful applications such as thermally stable down-converting layers for an LCD backlight, highly flexible composite layers, micro-patterned layers, and multi-deposited layers toward diverse display fields. In this presentation, we will overview the applicability of an AD process for the display applications, and report and discuss further our details.

9:50 AM

(GFMAT-248-2019) Bonding Mechanism of Ceramic Fine Particles on RTIC phenomenon of Aerosol Deposition Process

J. Akedo*[1]

1. National Institute of Advanced Industrial Science and Technology (AIST), Advanced Coating Technology Center, Japan

Deposition (AD) method is a unique approach for metal and ceramic coating, where solid state submicron metal and ceramics particles are accelerated by gas flow up to 100 - 500 m/s and then impacted onto a substrate. We found interesting consolidation phenomenon of

ceramic particles in this method over 20 years ago. During collision of fine particles and interaction with substrate, these ceramic particles, not only for oxide materials but also for non-oxide materials, formed thick, dense and hard ceramic layers at room temperature. No additional heating for solidification of ceramic powder was required. We named this phenomenon "Room Temperature Impact Consolidation (R.T.I.C)". When viewed as a powder forming process, this phenomenon is fundamentally different from a thermal spray coating and shock compaction in which raw material particles are brought into a molten or semi-molten state to obtain bonding between primary particles. Evidence for this is that atomic interdiffusion and amorphous layers are scarcely observed at the bonding interface between the particles formed by the AD process. In this presentation, the deposition mechanism of the AD process with RTIC phenomenon and comparison with other similar coating methods are explained.

10:10 AM

(GFMAT-249-2019) Liquid Phase Synthesis of Functional Nanoparticles Controlled in Size and Shape and their Application to Printed Electronics Technology

K. Kanie*[1]

1. Tohoku University, IMRAM, Japan

Electric circuits on substrates in smart devices are widely manufactured by a photolithography process. This process is advantageous for fabricating large-scale, high-quality integrated circuits. However, the multistaged masking and etching process requires expensive production systems and the use of harmful and environmentally undesirable chemicals. On the other hand, printed electronics (PE) technology has attracted a great deal of attention as an alternative eco-friendly and low-cost process to write electric circuits on flexible substrates with nanoinks. In this regards, functional nanoparticles-based inks have considerable potential as materials to fabricate next-generation devices. Up-to-date, we have investigated solvothermal synthesis of ITO, gallium-doped zinc oxide (GZO), and aluminium-doped zinc oxide (AZO) NPs with use of quaternary ammonium hydroxides. As a result, highly-crystalline ITO, GZO, and ATO NPs were successfully prepared through a one step process under solvothermal condition. Blue-coloured compacts of the TCO NPs obtained by the present method exhibited low resistivity. Nano-ink property of TCO NPs thus obtained has been also investigated for the development of TCO nanoinks. Furthermore, we have also developed metal nanoinks with low temperature sintering property applicable for PE technology.

G7: Ceramics Modeling, Genome and Informatics

Genome and Machine Learning

Room: Trinity I
Session Chair: Katsuyuki Matsunaga, Nagoya University

8:30 AM

(GFMAT-250-2019) Orbital-free density functional theory calculation combined with semi-local machine-learned kinetic energy density functional (Invited)

J. Seino*[1]; R. Kageyama[1]; M. Fujinami[1]; Y. Ikabata[1]; H. Nakai[1]

1. Waseda University, Japan

Density functional theory (DFT) is one of the most popular scheme for obtaining electronic states in molecules and materials. The total energy can be written as a functional of the electron density. The kinetic and exchange-correlation energies, which are components in the total energy, have approximate formulae because the exact expressions are unknown. For the kinetic energy (KE), the majority use the Kohn-Sham (KS) expression, which introduces a set of KS orbitals instead of using the explicit functional in terms of electron density. This is because the development of a practical KE density functional (KEDF) has been a difficult task. However, the orbital-free (OF-)DFT with the accurate KEDF has possibilities to realize further efficient calculations. The present study attempts to construct the KEDF using machine learning (ML). The present scheme adopts electron densities and their gradients as descriptors, and the KE density and its potential of KS as the objective value in atoms and molecules. A multi-layer neural network was adopted here for ML. These functionals are utilized for the optimization of electron density in the OF-DFT framework. The results showed that the ML KEDF provides closer KEs with the KS expression than conventional KEDFs.

9:00 AM

(GFMAT-251-2019) Design of new thermal barrier coating materials through high-throughput first principles calculations (Invited)

B. Liu*[1]; Y. Liu[1]

1. Shanghai University, China

High-throughput screening (HTS) has been increasingly developed as an efficient strategy on the seeking of materials with specific properties. High-throughput first principles calculations are performed on ABO_3 perovskites and $A_2B_2O_7$ pyrochlore-type rare-earth oxides for new thermal barrier coating (TBC) materials. We present systematic investigations comprised of multiple selection criteria to achieve the prediction of target materials. A database including mechanical/thermal properties of 190 perovskites and 94 pyrochlore is established. For ABO_3 perovskites, six perovskites are proposed as novel TBC materials with predicted thermal conductivities under 1.25 W/mK and good damage tolerance. In the case of pyrochlores, the machine learning algorithm is performed for the large family of pyrochlores and the parameters playing key role on mechanical/thermal properties are clarified. Besides, the expressions of focused mechanical and thermal properties are constructed. The adopted strategy and established database are expected to inspire the design of the next generation TBC materials and future structural material investigations.

9:30 AM

(GFMAT-252-2019) Phonon Engineering for tunable thermal properties of RE-silicate TEBC materials (Invited)

J. Wang*[1]

1. Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Advanced Ceramics and Composites Division, China

High-temperature capable cutting-edge T/EBC for SiC_f/SiC CMCs critically requested the better thermal properties of candidate materials. Rare earth silicates, typically including RE_2SiO_5 orthosilicates and $RE_2Si_2O_7$ pyrosilicates, are important EBC materials due to their excellent reliability in extreme combustion environments. There are crucial challenges to achieve lower thermal conductivity and better matched thermal expansion coefficients for their multifunctional TEBC perspectives. We have discovered unique characteristics of phonon behaviors in RE silicates. With the fundamental understanding of phonon anharmonicity, there emerges the opportunity to tailor their thermal conductivity and thermal expansion coefficient through strategic phonon engineering. The present work stimulates innovative design of multifunctional TEBC system for SiC_f/SiC CMCs.

Experiment Oriented Modeling
Room: Trinity I
Session Chair: Bin Liu, Shanghai University

10:20 AM

(GFMAT-253-2019) Electronic Structures at Dislocation Cores in Zinc Sulfide Showing Extraordinary Plastic Deformation

K. Matsunaga*[1]

1. Materials Physics, Nagoya University; Nanostructures Research Laboratory, Japan Fine Ceramics Center, Japan

Here we show that zinc sulfide single crystals with the zinc blend structure can undergo significantly large plastic deformation even at room temperature in complete darkness (Science (2018)). Under normal light or ultraviolet light exposure, zinc sulfide single crystals exhibit deformation twinning and immediately end up fracturing in a brittle manner with only a few percent of plastic strain. However, the single crystals exhibit plastic deformation up to a strain of more than 40% in compression when deformed in complete darkness. A high density of glide dislocations on {111} planes are generated in the samples deformed in darkness, so that the observed plastic deformation ability is caused by glide and multiplication of the dislocations. From DFT calculations, specific electronic structures localized around the dislocations cores are observed. A mechanism is that stability and mobility of the dislocations may be controlled by electrons or holes excited by external light.

11:00 AM

(GFMAT-254-2019) Modeling of PVD Process for Thermal Barrier Coating of Turbine Blades (Invited)

Y. Han*[1]; Y. Oh[1]; S. Lee[1]; H. Kim[1]

1. Korea Institute of Ceramic Engineering and Technology (KICET), Engineering Ceramic Center, Republic of Korea

The thermal barrier coating plays an important role in increasing the efficiency of the turbine engine. Especially, in order to develop a turbine engine that operates at a temperature of 1600°K or more, it is necessary to form a thermal barrier coating layer of a ceramic material by EBPVD. In this study, ZrO_2 with 8 mol% Y_2O_3 was coated on near-net shape turbine blades by EBPVD. FEM simulations were performed to develop a fixture for increasing thermal barrier coating uniformity. The simulation assumes that the ZrO_2 molecules are emitted from the melt produced on the ingot surface in cylinder form and deposited on the near-net shape turbine blade. As the process variables, the rotation speed and slope of the turbine blades and the distance from the ingot during the coating process were set. The turbine blades were rotated from 0 to 30 rpm and the slope was varied from 0 to 30 degrees. We also confirmed the influence of these variables on the TBC uniformity of near-net shape turbine blades.

11:30 AM

(GFMAT-255-2019) Core-rim structures as a hierarchical phase relationship developed by dopant re-distribution via sintering (Invited)

H. Gu*[1]

1. Shanghai University, School of Materials Science & Engineering, Materials Genome Institute, China

Phase relations and microstructure behaviors are usually two separate properties of sintered ceramics, one representing inherent structural uniformity and the other for native inhomogeneity, hence to engineer separately. Dopants as sintering aids form generally residual phases and stay at grain boundaries intergranular glassy film (IGF), while they could also dissolve into the primary ceramic structures although often in too low level to detect. In recent years, we have revealed re-distribution of dopant in the primary phases as core-rim structures, not only in oxides but also in nitrides, carbides and even borides. In most cases, solutions are uniform in either cores or rims, and the solution-reprecipitation process is associated with their development in separate stages of sintering. These core-rim structures lead to a hierarchical phase relationship establishing onto various levels of solid-solution of a same dopant, associated inherently with corresponding stages of sintering.

Monday, July 22, 2019

B2: Advanced Additive Manufacturing Technologies for Bio-Applications: Materials, Processes, and Systems

AM Technologies for Bio Applications I (Joint Session with G13)
Room: Trinity IV
Session Chairs: Soshu Kirihara, Osaka University; Cho-Pei Jiang, National Taipei University of Technology

4:30 PM

(BIO-001-2019) Fabrication of Bioceramic Implants by Stereolithographic Additive

S. Kirihara*[1]

1. Osaka University, Joining and Welding Research Institute, Japan

Bulky ceramic components including dendritic networks were geometrically built by stereolithographic additive manufacturing. Geometric patterns with periodic, self-similar, graded and fluctuated arrangements were created by computer aided design, manufacture and evaluation for effective modulations of liquids flow through biological scaffolds in artificial bones. Two dimensional cross sections were created through photo polymerization by ultraviolet laser drawing on a spread resin paste with ceramic particles, and three dimensional models were sterically printed by layer lamination with chemical bonding. Photo sensitive acrylic resins with hydroxyapatite and β-tricalcium phosphate of 3 μm in particle diameter at 50 vol.% were spread on a glass substrate with 10 μm in layer thickness by a mechanical knife edge. An ultraviolet laser beam of 355 nm in wavelength was adjusted from 10 to 100 μm in variable diameter and scanned on the pasted resin surface. Irradiation power was changed automatically from 10 to 200 mW to obtain enough solidification depth for layer by layer joining. Cross sectional patterns were laminated to create solid objects. Composite precursors were dewaxed and sintered. These bioceramic implants in centimeter order with graded and fluctuated patterns in micrometer order were designed and fabricated to realize vital fluid distributions and geometrical osteogenesis.

4:50 PM

(BIO-002-2019) Lithography-based Ceramic Manufacturing as tool for production of bioresorbable ceramic scaffolds

D. Bomze*[1]; C. Schmidleithner[2]; M. Schwentenwein[1]; D. Kalaskar[3]; J. Stampfl[2]

1. Lithoz GmbH, Austria
2. Vienna University of Technology, Institute of Materials Science and Technology, Austria
3. University College London, Division of Surgery and Interventional Sciences, United Kingdom

Treatment of bone defects involves frequently the application of scaffolds from suitable materials. It has been shown that bioresorbable materials are a good alternative to standard materials like titanium. Tricalcium phosphate (TCP), hydroxyapatite (HA) and blends thereof are bioresorbable ceramics which have been used in numerous medical applications. However, manufacturing defined and interconnected porous scaffolds of those materials is challenging. With lithography-based ceramic manufacturing (LCM) it is possible to produce complex scaffolds of adjustable pore geometry and size in highly reproducible manner. LCM is a slurry-based additive manufacturing technique that relies on the selective curing of photosensitive ceramic suspensions. Within the here presented work such scaffolds were produced and were analysed by light and scanning electron microscopy as well as computed tomography. High resolution and reproducibility show that the proposed approach is a suitable technique for the production of biomimetic scaffolds of bioresorbable ceramics. It could be shown that highly porous scaffolds could be produced with a minimum feature resolution around 150 μm for struts and pores as well as with a RSD of well below 3%. In addition, mechanical and biological testing was performed and the obtained results underline the good suitability for the usage of such structures as scaffolds.

5:10 PM

(BIO-003-2019) Innovative solutions in order to produce multi bioceramic implants by 3D printing

R. Gaignon*[1]

1. 3DCERAM SINTO, France

3DCERAM provides a unique expertise in the field of 3D ceramic printing. Applied to the biomedical market, the process allows the realization of eyeballs, bone substitutes or made-to-measure cranial implants in ceramics showing exceptional performance. Since 2017, 3DCERAM has developed a new multi material printer, in order to print several ceramics at the same time 3DCERAM has developed a unique 3D printing manufacturing process, based on laser stereolithography technology, to produce made-to-measure bioceramic cranial or jawbone implants. Enabling the production of implants with three-dimensional shapes in hydroxyapatite and tricalcium phosphates, materials widely renowned for their osteoconductive properties. Thanks to the unique process, 3DCERAM can produce bioceramic implants with porosity structured in 3 dimensions. The 3D printing process enables to control the location and geometry of porous areas and define a consistent diameter of pores. In the same implant, we can combine porous and dense areas. With the new hybrid (multi material) printing process, 3DCERAM can print HAP-TCP implants, with new complex designs and biomedical functions (you can target the HAP and TCP area). The 3D process uses the basic SLA process, while adding nozzle jets for the other ceramic (s) materials.

B4: Multifunctional Bioceramics: Current and Future Therapy

Multifunctional Bioceramics

Room: York B

Session Chairs: Miho Nakamura, Tokyo Medical and Dental University; Ahmed El-Ghannam, University of North Carolina at Charlotte

1:20 PM

(BIO-004-2019) Characterization and Control of Surface States of Metals and Ceramics (Invited)

T. Hanawa*[1]

1. Tokyo Medical and Dental University, Institute of Biomaterials and Bioengineering, Japan

To add biofunction to metals, surface modification is necessary. Surface modification can improve the tissue compatibility of the surface layer that is a metal oxide or ceramics. After micro arc oxidation (MAO), bone formation on titanium is accelerated by the formation of porous titanium oxide. Silver is easily contained in the surface oxide layer by the addition of silver in the electrolyte for MAO. Live bacteria decreased with increasing the amount of silver in the electrolyte and simultaneously calcification occurred in this silver amount. This result reveals that a dual-functional surface is formed on titanium by MAO. To clarify the effects of micron/nano hybrid topography on cell behavior and morphology, we investigated the adhesion of human mesenchymal stem cell (hMSC) to titanium surfaces covered by titanium oxide with topographies using a femtosecond laser. The different surface features had different effects on the differentiation of hMSC. The Hybrid surface topography promoted the differentiation of hMSC. In teh case of Yttria-stabilized zirconia, hydroxyl groups and phosphate groups on the surface were increased by immersion in water and Hanks' solution. The modest reaction of the surface may contribute to its superior reaction with soft tissues, as dental implants.

1:50 PM

(BIO-005-2019) Nonwoven polymer fiber mats-based scaffolds and bio-sensor substrates: Morphology, Structure, and Mechanical Properties (Invited)

P. Gouma*[1]

1. The Ohio State University, MSE, USA

Electrospinning holds particular promise for the synthesis of 3D scaffolds for regenerative medicine and for bio-sensor substrates because of the high surface area to mass ratio of the as-spun fibers and the exceptional control of the process over fiber diameter, morphology, and structure. However, one of the current limitations of the electrospinning process is its low production rate. The form of electrospinning that has shown the most promise for industrial application is needleless electrospinning of nanofibers on a free liquid surface. The lack of a defined nozzle allows for increased utilization of the polymer mat's own geometry. The microstructure of randomly distributed electrospun mats is correlated in this study with the mats' mechanical properties. The results are expected to inform the design of optimized mat configurations for improved biocompatibility.

2:20 PM

(BIO-006-2019) Bioactive Ceramic Dental Cements

C. Primus*[1]; R. Walsh[2]; K. Woodmansey[3]

1. Primus Consulting, USA
2. Advanced Endo of Texas, USA
3. St. Louis Univeristy, Center for Advanced Dental Education, USA

Tricalcium silicate cements have become the gold standard as bioactive dental cements, forming superficial hydroxapatite in vitro and in vivo. Such ceramic cements have been commercialized for use in pulp and endodontic therapy. These materials support the healing of injured pulps in children and adults and to restore roots, with the purpose of averting disease progression, including tooth extraction. Recent research has shown that calcium aluminate cement also has bioactive properties and is suitable for dental therapy. Analyses of dental cements will be given including x-ray diffraction, particle size distributions, discoloration and radio-opacity. The histological results comparing a tricalcium silicate and calcium aluminate cement in canine subjects will be presented, including contact with pulp tissue and in endodontic procedures.

2:40 PM

(BIO-007-2019) (Fe/Sr) co-doped biphasic calcium phosphate with tailored osteoblast cell functionality

S. Basu*[1]; A. Ghosh[2]; A. Barui[2]; B. Basu[1]

1. Indian Institute of Science, Materials Research Centre, India
2. Indian Institute of Engineering Science And Technology, India

The present study aims to quantitatively understand the impact of co-doping of Sr^{2+} and Fe^{3+} ions on the phase stability and cytocompatibility of the mixture of hydroxyapatite and tricalcium Phosphate, i.e biphasic calcium phosphate (BCP). Following sol–gel synthesis, co-doped BCP samples with different Sr/Fe dopant concentrations (2, 10, 20, 30, and 40 mol %) together with doped BCPs with single dopant (Sr or Fe) with similar compositions were calcined at 800 °C in air. The dopant content dependent crystallographic properties and phase stability of HA and TCP are quantitatively assessed by means of Rietveld refinement. In vitro cytocompatibility of co-doped samples has been assessed using mouse osteoblast cells. An important observation is that, while singular dopant of Sr/Fe at 20 mol % or higher amount reduces cell viability significantly, osteoblast viability is not compromised to any significant extent on Sr/Fe co-doped BCP, compared to undoped BCP. Our results indicate that one can tailor osteoblast functionality by controlling the co-dopant content. Cell morphological analysis supports extensive cell spreading on co-doped BCPs. An attempt has been made to correlate the variation in cellular response with HA/TCP ratio and ion dissolution behavior.

3:20 PM

(BIO-008-2019) Fiber-Reinforced Bioactive Composites for Implant Applications (Invited)

P. K. Vallittu*[1]

1. University of Turku, Biomaterials Science, Finland

Although metals, ceramics and particulate filler resin composites have successfully been used as implant biomaterials devices made out of these materials do not meet all surgical requirements. There has been a lot of development in the field of composite biomaterials and bioactive materials and more focus of implant development has been put to biostable composites as implant material. This presentation describes the structure and mechanism of function of biostable glass fiber reinforced composite (FRC) implants, which contains bioactive glass (S53P4). FRC with continuous glass fibers in a biostable thermoset resin matrix provide high strength and high toughness non-metallic biomaterial. By adding bioactive glass to the FRC implant, the implant supports osteogenesis and vascularization, and provide even antimicrobial properties for the implant. Structurally the implant mimics sandwich stucture of bone and it has been demonstrated in vitro, in vivo and clinically that the implant system induce osteogenesis even in large bone defects. Although the FRC implants and the material are used clinically in cranioplasties, further research is needed to demonstrate the most suitable implant designs for load-bearing applications for jaw bone reconstructions and orthopaedics.

3:50 PM

(BIO-009-2019) Application of synchrotron X-ray radiation for the analyses of biomaterials and biological tissues (Invited)

M. Uo*[1]

1. Tokyo Medical and Dental University, Advanced Biomaterials, Japan

Various metallic materials are widely used for medical and dental implants. Erosion and mechanical wearing of metal implants placed in the human body have been reported to be associated with localized and systemic problems. In addition, the oral and the respiratory mucosae are exposed to various dental restorative materials or inhaled foreign debris, then those would induce various symptoms. Therefore, the distribution and chemical state analyses of eroded metallic ions and foreign objects in tissues are important for the definite diagnosis. However, their contents are quite low, then, highly sensitive analysis method is required. Synchrotron radiation X-ray fluorescence (SR-XRF) and X-ray absorption spectroscopy (XAS) analyses are suitable method for the trace element analysis in the tissue specimens. We applied SR-XRF for the detection of the metallic elements eroded from the dental restoratives or implants and accumulated in oral mucosa. The trace element distribution and localization contained in the mucosa could be visualized. The inhaled foreign objects contained in lung tissues also could be identified by SR-XRF. Chemical state of eroded and accumulated trace elements from the metallic implant could be estimated using XAS. Those methods would provide the useful information for the medical diagnosis and also the estimation of the behavior of biomaterials in the tissues.

4:20 PM

(BIO-010-2019) Effect of different root canal filling materials in endo-perio lesions: Design and computational analysis

A. Purwar[1]; P. Pathak*[2]

1. Indian School of Business, India
2. Ramaiah University of Applied Sciences, Bengaluru, Department of Periodontics, India

Dental problems are mostly multifactorial in nature and, thus difficult to diagnose and treat. Among dental problems, Endo-perio Lesion (EP) is a complex disease entity which involves the tooth structure as well as the supporting periodontium. In this perspective, the current study was conducted with an aim to assess the effect of different root canal filling materials viz. gutta-percha, mineral trioxide aggregate (MTA) and Biodentine on EP Lesions. In the present work, a mandibular molar human tooth with lesion has been precisely modelled in consultation with a clinician. Then, four different finite element models representing different filler materials were developed. Next, the finite element models were validated with experimental data for a normal tooth under a defined (300N) masticatory load. Highly refined structured mesh with high fidelity second order elements was generated to perform the structural analysis. It was observed that stresses at the peri-apical area changed with the change in filler material type with the best result on the usage of biodentine. To the best of our knowledge, Biodentine as the filling material has not been investigated for its performance in a simulated study. In this perspective, our study intends to provide clinical inputs to dentists regarding the use of Biodentine as filling materials.

4:40 PM

(BIO-011-2019) Anisotropic crystal growth of dicalcium phosphate dihydrate by chemical micro-mist synthesis

T. Toshima*[1]; D. Yamashita[1]; S. Takamatsu[3]; M. Tafu[2]

1. National Institute of Technology, Toyama College, Department of Mechanical Engineering, Japan
2. National Institute of Technology, Toyama College, Japan
3. National Institute of Technology, Toyama Collge, Department of Applied Chemistry and Chemical Engineering, Japan

DCPD (dicalcium phosphate dihydrate, $CaHPO_4$-$2H_2O$) has been widely studied as a precursor of HAp (hydroxyapatite, $Ca_{10}(PO_4)_6(OH)_2$) which is a main component of living hard tissue. DCPD can be used for industrial applications such as implant agents and abrasives for toothpastes and DCPD is mixed with solvents or pastes. Therefore, controlling the morphology and orientation of DCPD are important because they become a controlling factor for miscibility and mechanical strength after conversion to HAp due to change the particles contact each other. Here we report anisotropic crystal growth of DCPD crystal by using chemical micro-mist synthesis. In this method, since the ion supply rate is suppressed, the ratio incorporated into the solid phase is significantly different from that in the normal solution missing process. Acicularization was confirmed by being preferentially incorporated into the negatively charged DCPD surface, particularly when the supply rate of calcium ions was suppressed. DCPD normally tends to grow in a flat plate structure perpendicular to the b-axis, or a petal structure in which the flat plate is aggregated. Therefore, the morphology is two-dimensional or pseudo three-dimensional structure. Since we succeeded in anisotropic growth in the one-dimensional direction, the potential as an admixture different from conventional powder properties is expected.

B7: Materials and Process Challenges to Upscale Fabrication of 3-D Tissue Constructs

Materials and Process Challenges to Upscale Fabrication of 3D Tissue Constructs

Room: York A
Session Chair: Markus Reiterer, Medtronic, PLC

1:30 PM

(BIO-013-2019) Nano-and Microfabricated Hydrogels for Regenerative Engineering (Invited)

A. Khademhosseini*[1]

1. University of California Los Angeles, Department of Bioengineering, USA

Micro- and nanoscale technologies are emerging as powerful tools for controlling the interaction between cells and their surroundings for biological studies, tissue engineering, and cell-based screening. Hydrogel biomaterials have been increasingly used in various tissue engineering applications since they provide cells with a hydrated 3D microenvironment that mimics the native extracellular matrix. We have developed various approaches to merge microscale techniques with hydrogel biomaterials for directing stem cell differentiation and generating complex 3D tissues. In this talk, I will outline our work in controlling the cell-microenvironment interactions by using patterned hydrogels to direct the differentiation of stem cells; including the fabrication and the use of microscale hydrogels for tissue engineering by using a 'bottom-up' and a 'top-down' approach. Top-down approach for fabricating complex engineered tissues involves the use of miniaturization techniques to control cell-cell interactions or to recreate biomimetic microvascular networks within mesoscale hydrogels.

2:00 PM

(BIO-014-2019) Robotic fabrication of tissues (Invited)

J. Hoying*[1]

1. Advanced Solutions Life Sciences, USA

Numerous challenges exist in the scaled manufacture of tissues for regenerative medicine and other applications. For example, each tissue has specialized and unique fabrication needs, reflecting its composition and function. Furthermore, the same tissue fabricated for different people will not be identical as intrinsic variations in anatomy, physiology, and genetics also influence outcomes. Thus, any solution translating current "by-hand" fabrication methods to meet these scale-out dynamics (many different products made once) must be agile and reliable. Consequently, we have brought forth an enabling tissue fabrication platform, called the BioAssembly™ Platform, utilizing a multi-axis robotic arm for the scaled fabrication of a spectrum of tissues and tissue microenvironments. With this biofabrication platform, we are developing a variety of fabrication approaches and applications related to bone, liver, microfluidic biosystems, tissue vascularization, and others. Each tissue fabrication strategy will utilize an automated, single-run process with the robotic arm performing the sequence of required, varied, tasks as instructed by the user console. With this platform, we envision technicians and clinicians utilizing patient-specific data, in combination with patient-specific cells and materials, to fabricate bespoke tissues with sufficient rigor and at a scale to meet the needs of numerous patients.

2:30 PM

(BIO-015-2019) In vitro tissue engineering by stimuli-responsive biomaterials (Invited)

M. Yamamoto*[1]

1. Tohoku University, Department of Materials Processing, Graduate School of Engineering, Japan

Stimuli-responsive biomaterials have been widely investigated not only as a drug carrier to enhance the efficacy of drugs in the body but also as a material to be utilized for stem cell culture as a tunable substrate. The physicochemical properties of the stimuli-responsive biomaterials could be altered in response to an external stimulus without cytotoxicity, such as temperature, light, magnetic field, chemical compounds. We designed stimuli-responsive biomaterials as a scaffold to be used for in vitro tissue engineering. In this presentation, I will introduce two types of hydrogel scaffolds with a stimulus-responsiveness to create a three-dimensional environment for cells in vitro. One is a sugar-responsive hydrogel scaffold that has been developed as a sacrificial template to introduce a defined vascular channel structure into a collagen hydrogel. The collagen hydrogel with a vascular channel structure could be utilized as a soft microfluidic device for disease researches. The other is an iron oxide nanoparticles-containing hydrogel as a magnetic responsive hydrogel scaffolds to be used for inducing spontaneous tubule formation of an epithelial cell in vitro. The epithelial tubule-like construct could function as a means to transplant cells with high bioactivities.

B12: Advanced Bioceramics and Clinical Applications

Advanced Bioceramics and Clinical Applications

Room: Trinity V
Session Chair: Xingdong Zhang, Sichuan University

1:30 PM

(BIO-016-2019) Bioceramic/polymer composites for tissue regeneration (Invited)

J. Chang*[1]

1. Shanghai Institute of Ceramics, Chinese Academy of Sciences, China

Silicate bioceramics have high activity in stimulating tissue regeneration. However, the pure bioceramics are often used only for bone regeneration and have limitations in clinical applications. Polymer materials have been widely studied due to good biocompatibility. Here, a novel injectable alginate (SA)-based hydrogel is developed by combining actions of divalent ions released from silicate bioceramics to crosslink SA. The gelling process and injectability of the hydrogel could be well controlled by adjusting the amount of silicate bioceramics in the composite hydrogels. In vitro results indicate that the composite hydrogel with optimized physicochemical properties is not only able to maintain the viability and proliferation of human bone marrow mesenchymal stem cells (hBMSCs) and human umbilical vein endothelial cells (HUVECs) but also shows stimulatory effects on osteogenic differentiation of hBMSCs and vascularization of HUVECs. In addition, in vivo results indicate that the SA/Aker composite hydrogel possesses osteoinductivity when it is injected subcutaneously in nude mice, which is the first time demonstration of osteoinductivity of silicate based biomaterials. Furthermore, when the composite hydrogel is applied in a chronic wound animal model, enhanced blood vessel formation and wound healing were observed suggesting the activity of the composite hydrogel for tissue regeneration applications.

2:10 PM

(BIO-017-2019) Polymeric brushite cement (P-DCPD) as a tool of local protein delivery

W. Ren*[1]; T. Shi[1]; D. C. Markel[2]

1. Wayne State University, USA
2. Providence Hospital, Orthopaedic Surgery, USA

Introduction: Development of new bioceramics as local protein delivery systems are challenging. The aim of this study was to evaluate the in vitro release of albumin from injectable self-setting polymeric brushite-forming cement (P-DCPD) and study the molecular interaction between albumin and P-DCPD matrix. Experimental: P-DCPD was prepared by reacting of calcium polyphosphate (CPP) gel with tetracalcium phosphate. The setting product is polymeric brushite (P-DCPD). FITC-albumin (a 66 kDa protein) was mixed with CPP gel before adding TTCP for setting (final 2 mg/g). FITC-albumin released was quantified by UV/vis spectrophotometer. Results and Discussion: A cumulative release of FITC-albumin from P-DCPD for more than 3.5 months was observed. A zero-order release of FITC-albumin is mainly due to the ionic interaction between albumin and the ionic polyphosphate backbone of CPP gel, which was validated by Raman analysis. Conclusions:The synergy between bioceramics and pharmacology has opened a wide field of possibilities, especially in the field of bone defect healing and the treatment of bone infections. Data generated from this study is very promising. We believe that P-DCPD represents unique injectable bone cement with a plethora of applications by including growth factors, antibiotics and other biomolecules.

2:30 PM

(BIO-018-2019) Rational Design of the Versatile Surface with Cells/Bacteria Recognition Capability and its mechanism

L. Wang*[1]; J. Chen[1]; Y. Wang[1]

1. South China University of Technology, School of Biomedical Science and Engineering, China

Biomaterial-associated infection remains a serious global problem and accounts for approximately 45% of all hospital-acquired infections. The antimicrobial biomaterials are in urgent need in clinic, especially that can selectively kill harmful bacteria. In the present study, we prepare a versatile surface on biomaterial by the rationally designed fusion peptide via 2D self-assembly. The fusion peptide has regular orientation on the surface. And this versatile surface can recognize bacteria to exhibit antibacterial activity and show improved biocompatibility to mouse bone mesenchymal stem cells (mBMSCs). Interestingly, by varying the structure of the recognition sequences in the fusion peptide, the versatile surface can further distinguish different bacterial strains from being broad-spectrum against both S. aureus and E. coli to being highly selective against only S. aureus. By all-atom molecular dynamics simulations (MD simulations), we find that this high selectivity towards specific bacterial strains is mainly caused by a less accessible surface area for the bacteria (BASA) in the AMP sequence of the fusion peptide. Furthermore, by the infective subcutaneous models on the SD rats, we demonstrated that the versatile surface can prevent bacterial infection in vivo (killing 96.2% of S. aureus) and improve the tissue-healing.

2:50 PM

(BIO-019-2019) Functional Bionic Hydrogels for Chondral and Osteochondral Regeneration

Y. Fan*[1]

1. Sichuan University, National Engineering Research Center for Biomaterials, China

Articular cartilage is an elastic tissue composed of chondrocytes and a large amount of collagenous extracellular matrix. Compared to other connective tissues, due to its avascular and aneural nature, cartilage has a very limited self-repair capacity once defected. Hydrogels are 3-dimensional networks of water-soluble or hydrophilic polymers that contain large quality of water. Many hydrogels possess good biocompatibility, suitable biomechanical properties, and desirable biodegradability, thus are found very important in numerous biomedical applications, including tissue engineering, drug delivery, and regenerative medicine. Hydrogels with various biofunctions have been reported to promote the cartilage growth and ECM secretion, and might be successfully applied in treating cartilage defects. In this work, the design, fabrication, and properties of bionic hydrogels are presented, focusing on the naturally derived hydrogels composed of biofunctional materials that are from cartilage sources. The chondral and osteochondral regenerative effects of hydrogels in vitro and in vivo are also introduced.

3:30 PM

(BIO-020-2019) Bio-inspired Nano-/micro- CaP Biomaterials and Scaffolds for Bone Interface Tissue Regeneration (Invited)

Y. Du[1]; J. Wang[1]; S. Zhang*[1]

1. Huazhong University of Science and Technology, Advanced Biomaterials and Tissue Engineering Center, China

Development of Tissue engineering and regenerative medicine evokes major challenges to fabrication of smart scaffolds with biomimetic interfaces. The current work shows a 3D construction of biomimetic gradient scaffolds for bone/cartilage tissue regeneration, including fabrication of nano-/micro-spheres, 3D selective laser sintering (SLS) of biomimetic gradient scaffolds, cytocompatibility evaluation and repair of bone/cartilage complex defect. The as-prepared microspheres exhibited uniform size, and gradient HA contents. Furthermore, the gradient microsphere-based 3D biomimetic scaffolds showed a multi-scaled porous structure, and adequate mechanical features. The SLS-derived biomimetic scaffolds can not only manipulate multiple stem cell behaviors, such as promoting cell adhesion, proliferation and inducing cell differentiation in vitro, but also induced vascularization of newly-formed tissue in vivo. Animal complex defect repair experiments demonstrated that significantly more bone was regenerated in the gradient multi-layer group than that in the control groups at week 6 and week 12. Histological analysis revealed the new bone integrated well with native tissue. At week 12, new cartilage was observed on the defect surface of the multi-layer group, with similar thickness and morphology, especially the characteristic zone distribution as native hyaline cartilage.

4:00 PM

(BIO-021-2019) Bioinorganic Angiogenesis (Invited)

J. Barralet*[1]

1. McGill University, Surgery, Canada

Blood supply is essential to new tissue growth, yet controling blood vessels in vivo is challenging beyond capillary invasion of pores in materials. This talk will consider how bioceramics interact with large diameter blood vessels and whether new agiosomes can be induced to form in them. There have been other attempts to induce luminal sprouting in blood vessels, most notably the arteriovenous loop (AVL) method. Here a vein graft is microsurgically stitched to an artery and thereby subjected to arterial pressure (20x than the thin walled vein experiences physiologically). It is thought this pressure drives neoangeogenesis and sprouting of the vein. This then can supply blood to a variety of scaffold and can generate considerable bone volumes. Our laboratory has been investigationg whether bioceamics alone have any capicity to induce vessel sprouting. Using 3D printed monetite ceramics made through powder printing phosphoric acid onto a tricalcium phosphate powder bed, hemi-cylindrical tubes were printed that could fit around blood vessels and be sutured together to enclose them. Blood vessel remodelling of the ceramic was monitred using X-ray microtomography and examination of histological sections. Our data suggest that bioceramics alone can induce angiogenesis on large diameter vessels without recourse to microsurgery offering a simple route to creating angoisomes that can be used in regenerative applications.

4:30 PM

(BIO-022-2019) Copper-containing silicate bioceramics for tumor therapy and tissue regeneration

Q. Yu*[1]; J. Chang[1]; C. Wu[2]

1. Shanghai Institute of Ceramics, Chinese Academy of Sciences, State Key Laboratory of High Performance Ceramics and Superfine Microstructure, China
2. Shanghai Institute of Ceramics, Chinese Academy of Sciences, Biomaterials and Tissue Engineering Research Center, China

Eliminating the residual tumor cells and simultaneously achieving the tissue regeneration are very important for cancer patients after surgery. Here, copper-containing silicate bioceramics were prepared with excellent photothermal effect for photothermal therapy of cancers and tissue regeneration ability for healing of surgery-caused tissue defects. $CaCuSi_4O_{10}$ nanoparticles (NPs) were synthesized and coated on the fiber surface. The composites could kill the tumor cells effectively at the early stage and promote healing of cancer surgery-induced wounds at the later stage. It was also found that the $CaCuSi_4O_{10}$-coated scaffolds released bioactive Cu^{2+} and SiO_4^{4-} ions to enhance angiogenesis and re-epithelization, thereby accelerating in vivo wound healing. Based on the results of bifunction with both tumor therapy and tissue regeneration capacities of copper-containing silicate bioceramics, copper silicate hollow microspheres (CSO HMSs)-integrated scaffolds were further designed for chemo-photothermal therapy and skin tissue regeneration. The composites showed synergistic antitumor performance and faster wound closure rates compared with the scaffolds without CSO HMSs. Therefore, the copper-containing silicate bioceramics may hold a great potential for cancer therapy and simultaneous healing of cancer surgery-induced defects.

4:50 PM

(BIO-023-2019) A Polydopamine/Bioceramic Multifunctional Composite Hydrogel for Infected Wound Healing

Q. Xu*[1]; J. Chang[2]

1. State Key Laboratory of High Performance Ceramics and Superfine Microstructure, Shanghai Institute of Ceramics, Chinese Academy of Sciences, China
2. Shanghai Institute of Ceramics, Chinese Academy of Sciences, China

Hydrogels have been extensively to admin the increasing demand of treating infectious wound. However, fabricating a hydrogel with excellent self-healing, adequate adhesiveness and efficient anti-bacterial properties still remains a challenge. Here, a multifunctional composite hydrogel mainly composed of dopamine polymer and copper-doped calcium silicate ceramic (Cu-CS) was prepared through the interaction between bioceramic and polymer components. The Cu-CS created an alkaline environment to oxidize the dopamine into polydopamine (PDA), while the generated PDA chelated the released Cu^{2+} ions from Cu-CS ceramic. The obtained hydrogel showed good self-healing property, and was self-healed immediately without any external stimuli, when it was cut apart and then put in contact again. The hydrogel also exhibited good adhesiveness on human skin both in dry and wet conditions. Moreover, the hydrogel had dual anti-bacterial activity resulting from NIR photothermal effect and controlled Cu^{2+} ions release, and the synergistic effect of both Cu^{2+} ions and photothermal property of the hydrogel resulted in high anti-bacterial efficiency. The in vivo study confirmed that the composite hydrogel inhibited bacterial growth and significantly enhanced infected wound healing and skin regeneration.

5:10 PM

(BIO-024-2019) Healing of osteoporotic bone defects by micro-/nano-structured calcium phosphate bioceramics

R. Zhao*[1]; S. Chen[1]; B. Yuan[1]; X. Chen[1]; X. Yang[1]; Y. Song[1]; H. Tang[2]; X. Yang[1]; X. Zhu[1]; X. Zhang[1]

1. Sichuan University, China
2. Capital Medical University, China

It is a particularly critical challenge to achieve enough bone regeneration in osteoporotic fractures with bone defects. In the present study, we designed a micro-/nano-structured calcium phosphate bioceramic composed of a nanoparticle-reinforced micro-whisker backbone (nwCaP). This sandwich-structured bioceramic exhibited a higher compressive strength, a suitable degradation rate and better cell attachment than traditional or intermediate bioceramics. In a rat model of osteoporotic bone defects, the nwCaP group showed a reduced fracture occurrence and an effective new bone substitution rate. The increased bone formation rate and greater amount of new bone formed within the defected area of the nwCaP group was revealed by the serum PINP level and histological staining. Moreover, a gene microarray study indicated that the promotion of osteogenesis might be attributed to selectively upregulated fibroblast growth factor 23 (FGF23) expression in cells co-cultured with the nwCaP bioceramic. Furthermore, the JAK2 signal pathway was confirmed to be involved in the nwCaP-induced elevation of FGF23 expression using primary osteoblasts derived from osteoporotic rats. Collectively, the findings suggested that the micro-/nano-structured bioceramic could enhance osteoporotic bone regeneration and presents a promising strategy for healing bone defects in osteoporosis.

Tuesday, July 23, 2019

B1: Innovations in Glasses for Healthcare Applications: A Symposium in Honor of Delbert E. Day

Delbert E Day Symposium: Session I

Room: York A/B
Session Chair: Leena Hupa, Åbo Akademi University

8:30 AM

(BIO-025-2019) Therapeutic bioactive glass and the challenge of ion incorporation (Invited)

J. Jones*[1]

1. Imperial College London, Department of Materials, United Kingdom

Bioglass was the first material found to bond with bone. Now it is termed as having the property “osteostimulation” because it can provoke cells to produce new bone through release of silica and calcium ions that stimulate bone cells. Delbert Day is a pioneer of use of biodegradable borate glasses and they are now used for wound healing applications. Glass can deliver the ions at a sustained rate because they are released as the glass dissolves. Silicate bioactive glasses originally had traditional modifier cations such as calcium and sodium. Substitution of these with alternative cations, such as strontium, lithium or zinc can provide therapeutic treatment of diseases such as osteoporosis, arthritis or cancer. Examples are zinc containing glasses that kill breast cancer cells but not healthy cells, at the same compositions. The glass can be delivered in the form of monodispersed nanoparticles that are internalised by cells. This talk will describe the challenges involved in getting cations into Stöber-like nanoparticles. Incorporation is easier in mesoporous nanoparticles but dissolution can be rapid. Network intermediates can control ion release. We have made great progress in making our Bouncy Bioglass, in terms of making glass flexible and 3D printing tough constructs for bone and cartilage applications. However, active ion incoporation is even more challenging, due to the low temperature processes.

9:00 AM

(BIO-026-2019) Influence of B for Si Substitution on Properties of Bioactive Phospho-Silicate Glasses (Invited)

D. S. Brauer*[1]; J. Brandt-Slowik[1]; L. van Wüllen[4]; J. Massera[3]; L. Hupa[2]

1. Friedrich-Schiller-Universität, Otto-Schott-Institut, Germany
2. Åbo Akademi University, Johan Gadolin Process Chemistry Centre, Finland
3. Tampere University, Faculty of Medical Sciences and Technology, Finland
4. Universität Augsburg, Institut für Physik, Germany

Bioactive glasses degrade in aqueous solutions, release ions and form an apatite surface layer that bonds to bone. However, they also crystallise easily, which can inhibit sintering. Here, we study the effect of B_2O_3 on the structure and properties of bioactive phospho-silicate glasses. Glasses based on 45S5 (46.1 SiO_2, 2.6 P_2O_5, 26.9 CaO, 24.4 Na_2O, mol%) were prepared by a melt-quench route; 1 to 25% of Si was replaced by B. FTIR and Raman spectroscopy showed a highly disrupted silicate network, with mostly Q^2 and some Q^3 groups. ^{31}P MAS NMR showed phosphorus present as orthophosphate. ^{11}B MAS NMR showed both 3-fold (80-90%) and 4-fold (10-20%) coordinated boron, with the relative amount of BO_4 increasing with B for Si substitution. T_g and crystallisation temperature decreased with substitution, owing to trigonal boron reducing network polymerisation. The processing window remained constant. pH upon immersion in Tris buffer increased with time but showed no changes with substitution. By contrast, in vitro apatite formation was accelerated with B for Si substitution, as shown by FTIR. SEM micrographs of discs treated in Tris buffer clearly showed the presence of an ion-depleted (silica gel) layer and an apatite surface layer. Taken together, results suggest that incorporation of borate can be used to tailor both thermal properties and degradation.

9:30 AM

(BIO-027-2019) Alkaline biodegradable implants for osteoporotic bone defects: Importance of microenvironment pH (Invited)

H. Pan*[1]; W. Liu[1]; X. Cui[1]

1. Shenzhen Institutes of Advanced Technology, Chinese Academy of Science, Center for Human Tissues and Organs Degeneration, China

In scenario of osteoporotic fracture, significantly higher activity of osteoclasts than osteoblasts may lead to continuous loss of bone in fracture/defect site. Impaired bone regeneration efficiency is the major barrier that influences endosseous implants to get a better performance, and this substantially increases the risk of a second fracture, nonunion, and aseptic implant loosening. Although great effects have been made, there are still no clinically approved biomaterials specifically tailored for applications in osteoporotic bones. The key issue for developing such biomaterials is to reestablish normal bone regeneration at the fracture site. Acid-base property could directly influence the behavior of bone cells, thus making it an important factor to modulate the unbalanced activity between osteoclast and osteoblast in osteoporotic conditions. More importantly, it is adjustable through implant biodegradation. Therefore, a rational strategy to reconstruct the regeneration balance in the fracture site is to regulate the micro environmental pH (μe-pH) through the application of biodegradable materials. We proposed that the μe-pH is an important and accessible factor which should be taken into consideration in the development of orthopedic biomaterials, in particular for repair of osteoporotic bone fracture/defect.

Delbert E Day Symposium: Session II

Room: York A/B

Session Chair: Delia Brauer, Friedrich-Schiller-Universität

10:20 AM

(BIO-028-2019) This Generation Biomaterials: Bioactive Borate Glasses in Clinical Use (Invited)

S. Jung*[1]

1. Mo-Sci Corporation, USA

The use of synthetic materials dates back nearly 100 years for treating osseous cavities in human tuberculosis patients and has evolved significantly in chemical composition, morphology, and application. One of the newest classes of biomaterials to be cleared by world regulatory agencies is the bioactive borate glasses. These materials have been allowed for use in orthopedics, spine, wound care, and veterinary medicine. The use of synthetic materials is increasing based on several factors including: excellent biocompatibility and clinical outcomes, low cost, low risk of disease transmission, anti infective properties, and the capability to make engineered shapes with controlled porosity. In addition to simply identifying materials that are biocompatible with human tissue, studies with respect to the materials themselves have been conducted to better our understanding of how to use them clinically. Local cellular effects that contribute to the healing process are being identified. Combining these new discoveries in biology with materials processing is the key to this generation of biomaterials.

10:50 AM

(BIO-029-2019) Bioactive Glasses for Regeneration of Large Segmental Bone Defects and Volumetric Muscle Loss (VML) (Invited)

Q. Fu*[1]; W. Jia[2]; H. Hu[2]; A. P. Tomsia[3]

1. Corning Incorporated, USA
2. Shanghai Sixth People's Hospital, Shanghai Jiaotong University, Department of Orthopedic Surgery, China
3. Lawrence Berkeley National Laboratory, Materials Science Division, USA

Injuries to either hard (bone) or soft (skin and muscle) tissues have profound consequence in healthcare. Regeneration of large segmental bone defects and volumetric muscle loss (VML) remains a challenge for materials and medical sciences. The current tissue engineering approach suffers from serious drawbacks: the availability of proper scaffold materials, the high cost of growth factors, and the lack of optimal strategies for growth-factor delivery. Here we show that, through the use of bioactive glasses, effective bone healing and defect bridging can be achieved in a rabbit femur segmental defect model without growth factors or stem cells. We further demonstrate that faster muscle regeneration can be achieved in a VML model in rats. Considering these promising results, bioactive glass may serve as a potentially simple, novel, and safe means to regenerate damaged bone and muscles.

11:10 AM

(BIO-030-2019) Controlling the dissolution kinetics of bioactive glasses: The key to tailored glass-based tissue engineering (Invited)

L. Hupa*[1]

1. Åbo Akademi University, Johan Gadolin Process Chemistry Centre, Finland

Bioactive glasses particulates are used mainly as bone filler materials. Today, increasing research efforts are paid to manufacture porous tissue engineering scaffolds of bioactive glasses. For the particulates and the scaffolds, the dissolution kinetics must be controlled to provide ideal conditions for the tissue regeneration. Over the years, various in vitro conditions have been used to assess the capability of different glasses to form the apatite-like surface layer characteristic for bioactivity. In this presentation, the information gained over the years from our in vitro tests is compared with the dynamic dissolution studies of bioactive glass particles and porous bodies. Further, the data are correlated with the observations from the in vivo experiments of selected bioactive glass compositions. The focus is to discuss how the in vitro data correlate with the capability of a particular bioactive glass to support tissue regeneration. The fluid flow rate through the sample affects the ion concentrations and pH of the interfacial solution. On the other hand, precipitation of apatite layer at the sample surfaces also affects the dissolution. A better understanding of the kinetics of bioactive glass dissolution and the reaction layer formation in dynamic liquids is the key to bioactive glass-based tissue engineering devices with a controlled and desired function.

11:30 AM

(BIO-031-2019) Design and characterization of bioactive glasses doped with tellurium

M. Miola*[1]; J. Massera[2]; A. Cochis[3]; L. Rimondini[3]; E. Vernè[1]

1. Politecnico di Torino, DISAT, Italy
2. Tampere University, Faculty of Medical Sciences and Technology, Finland
3. Università del Piemonte Orientale "A. Avogadro", Italy

Bioactive glasses have been deeply investigated for their ability to promote in vitro hydroxyapatite precipitation and in vivo bond with living bone. Moreover, several studies have been carried out to evaluate the effect of the introduction in the glasses network and the release of different active element, such as Sr, Cu, Ag, Ce and Zn (gene activating glasses) on tissue engineering and regeneration. Although Te is considered a non-essential trace element and shows a dose-related toxicity, its important biological effects, such as antibacterial and antioxidant properties, at low concentrations have been investigated. However, very few studies concerned the development of Te-doped biomaterials. In this work, a bioactive silica-based glass was doped with 1 and 5 mol% of TeO_2. The effect of Te introduction on thermal properties of the glass was investigated by means of DTA, evidencing a slight decrease of the characteristic temperatures for Te-doped glasses. FT-IR, SEM-EDS and Raman analyses, performed before and after the immersion of the glasses in simulated body fluid to estimate the effect of the Te insertion and its amount on the bioactivity, demonstrated that Te-doped glasses maintain the bioactivity. Cytocompatibility test and the evaluation of both antibacterial and antioxidant properties are in progress.

Delbert E Day Symposium: Session III

Room: York A/B

Session Chair: Showan Nazhat, McGill University

1:30 PM

(BIO-032-2019) Glasses and glass-ceramics for medical and dental applications (Invited)

W. Hoeland*[1]

1. private Person, retired, Liechtenstein

This lecture pays homage to the distinguished career of Prof. D.E. Day, a pioneer in the development of glasses for medical applications. At the same time, it is intended to bridge the gap between the glasses for human medicine and those for dental applications. Prof. Day, Prof. Hench and W. Höland explored the relationship between these two biomaterials systems in a joint publication some time ago. The present paper highlights the borat glass and yttrium-alumosilicate glass systems developed by Prof. Day, which are mentioned in this fundamental piece of work. The special features of these particular biomaterials are attributed to the role of their different glass phases. Glass-ceramic synthesis is also based on glass. High-strength and at the same time highly translucent dental glass-ceramics have been developed on the basis of alkali-silicate glasses with the addition of effective nucleation agents. Furthermore, specific properties have been combined in one material by making use of multifold nucleation and controlled crystallization processes. These development efforts have resulted in the production of glass-ceramics featuring special mechanical, optical and radiopaque properties.

2:00 PM

(BIO-033-2019) Effect of Mullite Whisker Addition on Properties of Lithium Aluminosilicate (LAS) Glass-Ceramics Prepared for Dental Restoration

Y. Zhang[1]; Y. Deng[1]; B. Wang[1]; J. Yang*[1]

1. Xi'an Jiaotong University, State Key Laboratory for Mechanical Behavior of Materials, China

Lithium aluminosilicate (LAS) glass-ceramics possess great potentials in dental materials for the excellent chemical stabilities and transparency. In this work, lithium aluminosilicate (LAS) glass-ceramics were prepared from lithium disilicate glass powder and mullite whiskers. Lithium disilicate glass powder (28.6Li–68.6Si–2K–0.8La, mol.%) with 5, 10 and 15 wt.% mullite whiskers were obtained. The effects of mullite on phase composition, microstructure, mechanical properties, coefficient of thermal expansion (CTE) and translucency were studied. Also, the mechanism for phase transformation and grain growth was discussed. The LAS glass-ceramic samples exhibited relative densities above 98% with main crystalline phases of lithium disilicate (Li_2Si2O_5, LD), lithium silicate (Li_2SiO_3, LM), and β-spodumene ($LiAlSi_2O_6$). The β-spodumene whiskers were in-situ synthesized through the reaction between mullite whiskers and glass matrix. The high β-spodumene content resulted in decreased lithium disilicate crystals content and increased lithium silicate, resulting in declined bending strength and improved fracture toughness. The formation of β-spodumene declined CTE and real in-line transmission of composites, while the specimens containing less than 10 wt.% mullite whiskers showed favorable translucency, which would suit applications in dental restoration.

2:20 PM

(BIO-034-2019) Biphasic calcium phosphate particles from dissolution-reprecipitation reactions of a borate glass

Y. Shen[1]; R. Brow*[1]

1. Missouri S&T, Materials Science and Engineering, USA

Delbert Day and his students showed that Ca-deficient hydroxyapatite (CDHA) particles could be produced by reacting soluble Ca-containing borate glass particles in phosphate solutions. The nano-porous CDHA particles retained the shape of the original glass particles, and could be hollow or solid, depending on the CaO-content of the precursor glass. In the present work, hollow CDHA microspheres were produced by reacting Li-Ca-borate glass microspheres in various phosphate solutions. The Ca-to-P ratio of the CDHA was controlled by the solution pH. When heated in air to 800°C, the CDHA transformed to nano-crystalline assemblages of hydroxyapatite (HA) and tricalcium phosphate (TCP), the ratio of which depended on the Ca-to-P ratio in the CDHA particles. The reactivity of these biphasic calcium phosphate (BCP) particles increased with an increase in their TCP-to-HA ratio, and the particles convert to nano-crystalline HA when exposed to simulated body fluids. Hollow, nano-porous, BCP and CDHA microspheres were implanted in calvarial defects in rats and after eight weeks, the BCP particles with a TCP:HA ratio of 70:30 were associated with the highest level of new bone growth. These same particles also supported the highest rate of new blood vessel formation in sub-cutaneous implants in rats.

2:40 PM

(BIO-035-2019) Manufacturing Porous Microspheres from Bioactive Glasses for Orthobiologics Applications (Invited)

I. Ahmed*[1]

1. University of Nottingham, Faculty of Engineering, United Kingdom

Manufacturing porous microspheres from bioactive glass materials can deliver significant advantages for bone repair and regeneration applications. Developing microsphere materials with larger external pores would be useful to accommodate cells (such as stem cells as an example). Producing microspheres with smaller pores could be utilised to encapsulate many other types of biological components such as drugs including small molecules, nucleic acids, proteins etc. We have successfully manufactured solid (non-porous) and highly porous microspheres from phosphate-based glasses, including borates and bio-silicate glasses. The current single stage lab-scale manufacturing process can produce materials between 1 – 3 kg/h. Solid (non-porous) glass microspheres of varying size ranges were successfully manufactured with over 95% efficacy of spherical morphologies. These microspheres contained surface and interconnected porosity and were produced at similar yields to the solid microspheres. Follow-on studies confirmed that human mesenchymal stem cells (hMSC) not only attached to the calcium phosphate glass microspheres, but also migrated within their pores. Studies have also shown that these materials can be delivered down 1mm and 2mm internal diameter needles. These newly developed novel biomaterials are currently being investigated for delivering the next generation of orthobiologic applications.

Delbert E Day Symposium: Session IV

Room: York A/B

Session Chair: Richard Brow, Missouri S&T

3:20 PM

(BIO-036-2019) Bioactive sol-gel derived borate glasses (Invited)

W. C. Lepry[1]; E. Rezabeigi[1]; S. N. Nazhat*[1]

1. McGill University, Mining and Materials Engineering, Canada

Borate glasses are chemically less durable than silicate glasses and convert more rapidly to carbonated hydroxyapatite (CHA). Sol-gel processing also offers increased compositional flexibility, homogeneity, and reduced processing temperatures, which impact glass dissolution rates and potentially widen its applications. We have demonstrated that sol-gel derived borate glasses (SGBGs); e.g., a boron substituted Bioglass 45S5 formulation; [(46.1)B_2O_3-(26.9)CaO -(24.4)Na_2O-(2.6)P_2O_5; mol%] with at least two-orders of magnitude greater specific surface areas and pore volumes compared to melt-derived equivalents, have higher solubility and ion release rates and at least a 25-fold increase in CHA conversion rate, in vitro. This CHA formation is also associated with an increase in pH upon SGBG dissolution, a feature that can be used to fibrilize and mineralize injectable and 3D-printable dense collagen hydrogels. Acid-solubilized collagen molecules self-assemble in the presence of dissolving SGBGs without the use of NaOH, which then rapidly (< 2 hours) mineralize in simulated body fluid. This latest breakthrough enables the development of bespoke bioink formulations that can be used with a novel 3D printing technology. This can enable the building of rapidly mineralizable tissue-mimicking structures with varying architectures to mimic native protein fibril density and alignment, as well as cell loading and density according to the intended use.

3:50 PM

(BIO-037-2019) Bioactive Silicon Oxycarbide Glasses with Highly Connected Network

E. Ionescu*[1]; S. Sen[2]; F. Xie[1]; G. Mera[1]; I. Gonzalo[1]; A. Navrotsky[3]; A. R. Boccaccini[4]

1. Technical University Darmstadt, Materials Science, Germany
2. University of California, Davis, USA
3. University of California, Davis, Peter A. Rock Thermolab and NEAT ORU, USA
4. University of Erlangen-Nuremberg, Institute of Biomaterials, Germany

In the present work, alkaline and alkaline earth metal bearing silicon (boro)oxycarbide glasses were prepared from polysilsesquioxane-based single-source precursors and investigated concerning their network architecture and thermodynamic stability. The obtained glasses were shown to be bioactive despite their high network connectivities (i.e., > 5, much higher than that of vitreous silica, which itself is not bioactive). It seems that strong carbon-for-oxygen substitution in these glasses significantly improves their thermal and mechanical properties due to very high network connectivity; whereas at the same time, the bioactivity can be provided via minor depolymerization of the network (e.g., via alkaline/alkaline earth metals modification) in combination with an open network architecture. Silicon oxycarbide-based glasses can be considered as interesting model compounds for developing advanced design concepts for highly-connected bioactive glasses, which may be exciting material candidates for e.g. load-bearing applications. Such a rational design of these materials may allow for significantly improving their performance and expand the scope of their applications.

4:10 PM

(BIO-038-2019) Effect of TiO_2 on sinter-crystallisations of Nepheline glasses for Dental applications

A. Alzahrani*[1]

1. College of Dentistry, Taif University, Dental Physical Sciences and Technology Unit, Saudi Arabia

The addition of TiO_2 in certain surface crystallised glasses known to act as nucleation agents to promote the development of a high density of internal nucleation sites and used as a key to the achievement of controlled crystallisation (Duke et al., 1967). The aim of this study was to investigate the effect of TiO_2 on the sinter-crystallisations behaviours of a newly developed nepheline ($NaAlSiO_4$) glasses. Three glass compositions based on multicomponent system containing sodium-magnesium-alumina-silicate were synthesised using melt-quench method. Glasses were named after their TiO_2 molar percent contents, Ti3, Ti6 and a titanium free glass Ti0. Experimental glasses were ground into fine powders (D50 around 25 μm) then heat-treated via sinter-crystallisation route at the exact crystallisation schedule. Glasses and glass-ceramics were characterized before and after crystallisation using differential scanning calorimetric (DSC), Dilatometry (DIL), X-ray diffraction (XRD), scanning electron microscopy (SEM) and nuclear magnetic resonance (NMR). This paper will discuss the effect of TiO_2 on the sinter-ability and crystallisation of the newly developed nepheline glasses in term of; 1) the glass ability to be sinter-crystallised into dense monolithic glass-ceramics, and 2) changes in thermal behaviours and the residual glassy matrix after crystallisation.

B2: Advanced Additive Manufacturing Technologies for Bio-Applications: Materials, Processes, and Systems

AM Technologies for Bio Applications II

Room: Trinity IV
Session Chairs: Naoyuki Nomura, Tohoku University; Qiang Fu, Corning Incorporated; Hui-suk Yun, Korea Institute of Materials Science

8:30 AM

(BIO-039-2019) 3D Printing of Bioactive Glasses for Improved Healthcare (Invited)

Q. Fu*[1]; A. P. Tomsia[2]

1. Corning Incorporated, USA
2. Lawrence Berkeley National Laboratory, Materials Science Division, USA

The need for implants to repair large bone defects is driving the development of porous scaffolds of requisite mechanical strength and reliability in vivo. Recent developments in the use of design principles and novel fabrication technologies are paving the way for the creation of synthetic scaffolds with promising potential for reconstituting bones in load-bearing sites. This talk reviews the state of the art in the design and fabrication of bioactive glass scaffolds that exhibit improved mechanical properties for load-bearing bone repair. The impact of glass composition, rheological properties of glass ink and the impact of polymeric coating on the final performance of 3D-printed scaffolds will be covered. Future research toward the improved designs that provide strong, tough scaffolds with microstructures conducive to bone ingrowth, and evaluation of these scaffolds in large animal models will be discussed.

9:00 AM

(BIO-040-2019) 3D printing of PLA/Calcium Silicate hybrid filament for load-bearing regenerative medicine

F. Shirazi*[1]; P. Lotfi[2]; S. Rahmati[2]

1. Confederation College, Canada
2. Science and Research University, Islamic Republic of Iran

Given its highly printable and biocompatible properties, PLA can be potentially considered as a great promise material in the field of bone tissue engineering. PLA suffers from lack of bioactivity and fast degradation, however incorporation of bioactive nanoceramics can improve the mechanical and biological properties of PLA. Apart from the novelty of making the hybrid filament, current study refers to FDM 3D printing of PLA/Calcium silicate (CS) filament for regenerative medicine applications. In vitro-cell viability of human mesenchymal stromal cells (hMSCs) on printed specimens was assessed by using the MTT assay. The cell-adhesion results showed that hMSCs were viable at variable time points on the PLA/CS 3D printed samples. The results also confirmed that the degradation of PLA was remarkably improved by introducing of CS into the polymer matrix while the apatite formation was significantly enhanced with soaking the samples in simulated body fluid (SBF). Moreover, the results confirmed that the mechanical properties of printed samples were increased due to the presence of CS in the structure of polymer matrix.

9:20 AM

(BIO-041-2019) Applying three-dimensional slurry printing technology to fabricating root-analogue implant

H. Hsu*[1]; S. Lee[1]; C. Jiang[2]

1. National Yang-Ming University, Department of Dentistry, Taiwan
2. National Taipei University of Technology, Mechanical Engineering, Taiwan

Screw-type implants are highly unnatural in form and unfit the tooth socket. It prones to peri-implantitis and plaque accumulation because implantation surgery involves drilling into healthy bone, filling gaps between implant and bone. This study proposes to use a three-dimensional slurry printing technology to fabricate the root-analogue implant and discuss the fitness of tooth socket. The mechanical properties such as flexural strength and hardness are evaluated according to the clinical requirement. The experimental result shows the volume enlarge ratio is 1.21 and tolerance of socket fitness is less than 120 μm. The Hardness is 1556 Hv but the flexural strength is 682 MPa which is less than the clinical requirement of 800 MPa. Further study focuses on optimization of sintering parameter to meet the requirement of flexural strength.

9:40 AM

(BIO-042-2019) Low temperature fabrication of self-setting bioceramic scaffolds using material extrusion process

H. Yun*[1]

1. Korea Institute of Materials Science, Republic of Korea

Material extrusion (ME) is one of representative additive manufacturing processes in which material is selectively dispensed through a nozzle. ME processes are widely applied to produce 3D porous bioceramic scaffolds in bone tissue regeneration. The ceramic scaffolds are generally sintered after control 3D structures by ME process to achieve the desired mechanical properties. However, the sintering process often leads to shortcomings in biofunctional performance of ceramic scaffolds because functional materials such as biomolecules and drugs are easily denatured by heat and therefore cannot simultaneously print with ceramics. Our group is the first to suggest a novel ME process for creation of bioceramic scaffolds without sintering, to enhance the biofunctionality of scaffolds while retaining mechanical strength. Mechanical stability of the bioceramic scaffold was achieved by adapting a self-setting reaction after ME process rather than using a sintering process. Compressive strength could control up to 30 MPa. Both final crystal state and biodegradability of scaffolds were also controlled by adjusting self-setting reaction. This process could be applied to fabricate various types of bioceramic scaffolds with biofunctional materials, such as osteoblast cells, drugs, biomarkers, and proteins, thereby providing highly functional scaffolds for effective bone tissue regeneration.

10:20 AM

(BIO-043-2019) Introduction on three-dimensional slurry printing technology and its application in digital dentistry (Invited)

C. Jiang*[1]; S. Lee[2]

1. National Taipei University of Technology, Mechanical Engineering, Taiwan
2. National Yang-Ming University, School of Dentistry, Taiwan

The mass customized demand has accelerated the rapid revolution in additive manufacturing technology. Manufacturing artificial teeth meet the needs of mass customizations because each person's teeth are different in appearance. This paper introduces the development of digital dentistry technology including digital scanning, digital design, digital manufacturing, and preclinical validation. Digital scanning contains reverse scanning of the plaster model, intraoral scan and measurement of the marginal gap. Digital manufacturing mainly introduces the principle of three-dimensional slurry printing (3DSP) technology and process parameters. The material used is zirconia oxide. The composition of zirconia slurry and sintering parameters are optimized to obtain high flexural strength and hardness with the stable phase microstructure. A dental coping model is proposed as the benchmark. It is made by the dental CAD/CAM and 3DSP to compare the mechanical properties and accuracy. The results demonstrate that the dental coping made by the 3DSP meets the FDA's requirements but the flexural strength is lower than that of the CAD/CAM.

10:50 AM

(BIO-044-2019) Microstructure and mechanical properties of additively manufactured Zr-1Mo alloy for biomedical applications (Invited)

N. Nomura*[1]

1. Tohoku University, Graduate School of Engineering, Department of Materials Processing, Japan

To decrease artifacts in magnetic resonance images and realize tailor-made medical devices, low magnetic Zr-1Mo alloy were fabricated by powder bed fusion process with fiber laser (L-PBF). Pore distribution of as-built Zr-1Mo alloy were observed by scanning electron microscope. Phase constitution was analyzed by X-ray diffraction. Microstructure was examined by transmission electron microscope. The magnetic susceptibility and mechanical properties were evaluated by magnetic susceptibility balance and tensile test, respectively. Process map on the pore distribution revealed that aligned, randomly distributed, and big size pores were formed depending on the scanning parameters and the formation mechanisms were different among them. Impurities and crystallographic orientation had influences on the mechanical properties of the as-built alloy rather than porosity. The magnetic susceptibility of the as-built Zr-1Mo alloy was lower than that of Ti-6Al-4V alloy, thus L-PBF can be applicable to the fabrication process for the low magnetic Zr-1Mo alloy.

11:20 AM

(BIO-045-2019) Load Bearing 3D Printing Bioceramic for Bone Regeneration via Negative Thermo-Responsive Hydrogel Forming

C. Wang*[1]; Y. Su[2]; S. Lin[2]; Y. Wang[3]; C. Lin[1]

1. Kaohsiung Medical University, Department of Medicinal and Applied Chemistry, Taiwan
2. Kaohsiung Medical University, Kaohsiung Medical University Hospital, Taiwan
3. Kaohsiung Medical University, School of Dentistry, Taiwan

The porous biphasic bioceramics of hydroxyapatite/β-tricalcium phosphate can promote osteo-conduction during new bone formation in clinincal use. The brittle nature of porous bioceramic substitutes cannot match the strength of bone, which limits the use of these materials for clinical load-bearing applications. The novel methods can enhance mechanical properties are mainly based on the admixture of a combustible reverse negative thermo-responsive hydrogel (poly(N-isopropylacrylamide; p(NiPPAm), which burns away during sintering in the resulting object. The p(NiPPAm) base hydrogel undergoes a reversible lower critical solution temperature phase transition from a swollen hydrated state to a shrunken dehydrated state, losing huge amount of water volume. This method can be regarded as functioning in a manner similar to the cold isostatic press (CIP) step before the powders sintering densification process. In other words, sintering densification is expected via free volume contraction, which will increase the mechanical properties after the formation of the bicontinuous phase bioceramics. However, this novel method have obtained the compressive strength of the sintered body of bioceramic was about 20 MPa and its porosity near to 40%. We are going to evaluate bone regeneration of calvarial defects from rabbits and high tibial osteotomy from pig.

11:40 AM

(BIO-046-2019) 3D cell printing of volumetric construct using tissue-derived bioink

Y. Choi*[1]; H. Yun[2]; D. Cho[3]

1. Korea Institute of Materials Science, Engineering Ceramics Research, Republic of Korea
2. Korea Institute of Materials Science, Republic of Korea
3. Pohang University of Science and Technology(POSTECH), Mechanical Engineering, Republic of Korea

Tissue-derived bioinks, also known as decellularized extracellular matrix (dECM) bioinks, have been widely investigated for the 3D bioprinting of tissue and organs because they represent a native microenvironment that can guide cell migration, proliferation, differentiation, and maturation. While dECM bioinks can facilitate robust tissue regeneration, building of volumetric constructs is challenging due to their low printability and weak mechanical properties. Here, we demonstrate a granule-based printing reservoir that facilitates 3D bioprinting of large-volume constructs using soft dECM bioinks without chemical modification or loss of structural fidelity. The dECM bioinks and cells were extruded into a granule-based printing reservoir, allowing the fabrication of free-standing tissue construct that maintained its position in between the granules without being affected by gravity. We found that 3D bioprinted dECM constructs maintained high cell viability and functionality and promoted de novo tissue regeneration in vitro and in vivo. This novel printing method can broaden the application of dECM bioinks and facilitate the fabrication of complex 3D cell structures with high biofunctionality; this will be particularly useful in the field where complex 3D tissue structures are needed.

12:00 PM

(BIO-047-2019) Nanoclay Impregnated Target Specific Crosslinked Biopolymer for Control Drug Release

S. Sagar Iqbal*[1]; N. Ehsan[2]

1. University of the Lahore, Department of Physics, Pakistan
2. University of the Lahore, Department of Chemistry, Pakistan

Owing to remarkable advancement in field of controlled drug delivery, many of drugs have uncontrolled side effects potentially due to undesired interactions of drug with other organs that are not the desired target of administered drug. Certainly, there is an increasing concern in development and usage of biopolymers and advanced skills that can lessen the reliance on artifact energy and transfer to a viable resources. Biopolymer based novel pH-sensitive hydrogels were prepared using natural chitosan, gelatin and synthetic PVP polymers in the presence of silane crosslinker. Tetraethylorthosilicate was selected as a crosslinker due to its nontoxic nature and different amounts of kaolin used to study its impact on physical and chemical properties of newly synthesized GK hydrogels. The swelling behavior of synthesized hydrogels were investigated in water, buffers, and ionic solutions. In water swelling ratio decreased with increase in concentration of clay. All hydrogels represent maximum swelling in acidic pH and low in basic and neutral pH. This specific pH responsive behavior at neutral pH made them suitable for injectable controlled drug delivery. Levofloxacin successfully loaded on GK hydrogel to study its released mechanism.

B3: Clinical Translation of Biomaterials and Biophysical Stimulation

Modern Biomaterials

Room: Trinity V
Session Chairs: Bikramjit Basu, Indian Institute of Science; Shalini Gupta, Indian Institute of Technology Delhi

11:20 AM

(BIO-048-2019) Bioresorbable Electronics

J. Rogers*[1]

1. Northwestern University, Materials Science and Engineering, USA

A remarkable feature of modern integrated circuit technology is its ability to operate in a stable fashion, with almost perfect reliability, without physical or chemical change. Recently developed classes of electronic materials create an opportunity to engineer the opposite outcome, in the form of 'transient' devices that dissolve, disintegrate or otherwise disappear at triggered times or with controlled rates. Water-soluble transient electronics serve as the foundations for interesting applications in zero-impact environmental monitors, 'green' consumer electronics and bio-resorbable biomedical implants. This presentation describes the foundational concepts in chemistry, materials science and assembly processes for bioresorbable electronics in 1D, 2D and 3D architectures, the latter enabled by approaches that draw inspiration from the ancient arts of kirigami and origami. Wireless sensors of intracranial temperature, pressure and electrophysiology designed for use in treatment of traumatic brain injury and nerve stimulators configured for accelerated neuroregeneration provide application examples.

B9: Advances in Production Methods and High-Performance Materials for Dental, Oral and Maxillofacial Applications

High-performance Materials for Dental, Oral, and Maxillofacial Applications

Room: Trinity V
Session Chair: Roger Narayan, NC State University

8:30 AM

(BIO-049-2019) Bone regeneration assisted by highly pure calcite ceramics: Artificial Coral as a new bone augmentation material

S. Umemoto*[1]; M. Tajika[1]; H. Unuma[2]; T. Furusawa[2]

1. Shiraishi Central Laboratories CO., LTD., R&D, Japan
2. Yamagata University, Chemistry and Chemical Engineering, Japan

Porous and monolithic $CaCO_3$ originated from marine creatures has been clinically used as effective bone augmentation material (e.g. Biocoral^{TM}). In contrast to other calcium phosphate-based artificial bones (HA, b-TCP), $CaCO_3$-based ones have been harvested from marine corals in spite of the risk of extermination of the coral and the pollution of the marine environments. The major reason for that has been that $CaCO_3$ cannot be sintered due to its high tendency to thermal decomposition. The present authors, however, have succeeded in densely sintering highly pure (> 99.99%) $CaCO_3$ (calcite) into either porous or dense ceramics. In this study, we fabricated porous $CaCO_3$ scaffold (60 - 85% porosity, 200 - 500 mm in pore diameter) and implanted them into the bone defects in the calvaria of SD rats. As compared with the control scaffold (b-TCP), $CaCO_3$ scaffold promoted faster bone formation and bone maturation in exchange for its faster resorption. These results imply that sintered $CaCO_3$ ceramics can be a good bone augmentation material especially to be used in dental and maxillofacial surgeries where prompt substitution of materials with bones is required.

8:50 AM

(BIO-050-2019) Comparison load –bearing capacity of three manufacturing methods of ultra-thin occlusal veneers

A. Ioannidis[2]; D. Bomze*[1]; C. Hämmerle[2]; J. Hüsler[3]; O. Birrer[2]; S. Mühlemann[2]

1. Lithoz GmbH, Austria
2. University of Zurich, Clinic of Fixed and Removable Prosthodontics and Dental Material Science, Switzerland
3. University of Bern, Institute of Mathematical Statistics and Actuarial Science, Switzerland

Ultra-thin occlusal veneers (UTOVs) are a suitable treatment alternative in case of extensive tooth substance loss. Compared to the standard treatment route for tooth substance loss where a full-crown restoration, UTOVs are much less invasive treatments saving most of the native tooth substance. Classical production methods for UTOVs are either milling of zirconia or pressing of lithium disilicate. Lithography-based Ceramic Manufacturing (LCM), an additive manufacturing process for high-performance and bioresorbable ceramics, offers a new possibility for the manufacturing of those highly delicate dentures. LCM shapes ceramic slurries, which consist of ceramic particles dispersed in organic photocurable binder matrix, in a layer-by-layer process by using visible light. Beside freedom of design other benefits of LCM compared to subtractive methods are very efficient material usage, high resolution and the capability to generate very delicate features down to 100 µm. Within the presented study, LCM technology is evaluated towards its technical capability for producing UTOVs made of zirconia. Furthermore, the strength of three sets of differently manufactured dentures are compared after simulated aging in chewing simulators indicating the suitability of using additive manufacturing as technique for producing patient-specific occlusal veneers in high quality.

9:10 AM

(BIO-051-2019) Making Bijels-derived Bicontinuous Structures for Tissue Engineering Applications Using a Newly Developed Technique

J. Li[1]; H. Sun[1]; M. Wang*[1]

1. The University of Hong Kong, Department of Mechanical Engineering, Hong Kong

Bicontinuous structures with interconnected pores are attractive for tissue engineering applications but making good bicontinuous structures is a challenge. Bicontinuous interfacially jammed emulsion gels ("bijels") are a recent discovery and can be used as templates to produce bicontinuous structures. However, common fabrication techniques for bijels involve complicated processes and are time-consuming. In our recent research, a greatly simplified method that can fabricate large three-dimensional bijels was developed. In this study, using this method, hexanedioldiacrylate (HDA)-water bijels were made first. HDA was then photo-crosslinked. The domain size in bijels could be changed by varying CTAB concentration in bijels fabrication. The "bijels" with crosslinked HDA were subsequently immersed into a Na-alginate solution for substituting water phase by alginate, taken out and immersed in a $CaCl_2$ solution for crosslinking alginate, thereby forming bijels-derived hybrid hydrogel membranes with bicontinuous structures. Various techniques were used to study bijels and bijels-derived membranes. In vitro biological experiments were also performed. SEM and confocal microscopy revealed the bicontinuous phases. Cell viability tests showed the bicontinuous structures were biocompatible, and MTT results indicated good cell proliferation on these bicontinuous structures.

9:30 AM

(BIO-052-2019) Electrocatalytic disinfection of Staphylococcus aureus biofilms using n-type TiO_2 nanotubes

H. Malik*[1]; K. Carlson[1]; S. K. Mohanty[2]; J. Colombo[3]

1. University of Utah, Metallurgical Engineering, USA
2. University of Utah, Chemical Engineering, USA
3. University of Utah, Dentistry, USA

In this study we exploited the electrocatalytic properties of n-type TiO_2 nanotubes for effective shredding of Staphylococcus aureus biofilm. Staphylococcus aureus is a dangerous bacteria, causing skin infections, pneumonia and bone infections. The defect laden TiO_2 ceramic structures provide large surface area, high disinfection, and possibilities for localized treatment. The electrochemical behaviour of the TiO_2 electrodes was determined by cyclic voltammetry and electrical impedance spectroscopy. The electrocatalytic study on the biofilms was done by assembling a device based on TiO_2 electrode as the anode and platinum as the cathode. The disinfection of the biofilms was done in a voltage range of 2-6 volts. This study determined the mechanism behind shredding of biofilm using defect laden TiO_2 electrode, their interaction with the polymer matrix, and the bacteria constituting the biofilms. The efficacy of electrodes was tested in simulated body fluids.

B11: Material Needs for Medical Devices

Material needs for Medical Devices I

Room: Trinity V
Session Chairs: Masamoto Tafu, National Institute of Technology, Toyama College; Masanori Kikuchi, National Institute for Materials Science (NIMS)

1:30 PM

(BIO-053-2019) Bouncy 3D printable bioglass for cartilage regeneration (Invited)

J. Jones*[1]

1. Imperial College London, Department of Materials, United Kingdom

Clinicians need bioactive materials that can share load with cartilage (including providing a bearing surface), while recruiting cells from the underlying bone marrow, before they biodegrade at a controlled rate. Such devices are not yet available, but they could be, using our new hybrid biomaterials. Hybrids have nanoscale co-networks of inorganic glass and organic components, e.g. sol-gel silica and biodegradable polymers. We now have hybrids that can "bounce" and self-heal. The hybrids are ideal for 3-D printing inks, which can yield bespoke scaffold architectures. Osteochondral devices can now be 3D printed that stimulate articular cartilage production and also provide the bearing surface with tribology similar to native cartilage, e.g. coefficient of friction tested against living collagen. Mechanical properties and degradation rate are determined by the amount of polymer and degree of cross-linking. Self-healing is due to polymer chain mobility and hydrogen bonds allowing crack bridging. When our hybrids are printed to have 200 mm pore channels, they provoke chondrocytes to produce type II collagen matrix, Sox9 and Aggrecan. Importantly, they do not produce type or type X collagen. Bone marrow stem cells showed similar results. Use of star polymers enables development of hybrids that degrade under action of enzymes.

2:00 PM

(BIO-054-2019) Exposure models in biomedical applications (Invited)

D. Saylor*[1]

1. USFDA, USA

The materials that comprise medical products contain substances that can be transferred to patients during use. Patient exposure to these substances may be desirable, such as in drug delivery applications, but more generally, there is concern for adverse health effects if a chemical is released in sufficient quantities. Historically, the likelihood for adverse health effects has been evaluated primarily through animal testing. However, toxicological risk assessment approaches are increasingly being used, potentially obviating the need for extensive animal testing. A critical component of these approaches is exposure assessment, yet exposure data are often unavailable, i.e. the amount of a chemical that is released from the product and taken up by the patient. Mass transport/transfer models provide a promising means to establish clinically relevant exposure estimates. However, the use of these models to support toxicological risk evaluations is virtually non-existent, largely due to challenges with parameter specification and validation. This presentation will provide an overview of exposure models and their use in biological risk evaluation of medical products, including: 1) potential benefits and current use in regulatory applications; 2) types of models that can help inform toxicological risk assessments; 3) challenges associated with use in regulatory decision making; and 4) strategies to overcome these challenges.

2:30 PM

(BIO-055-2019) Improvement of reactivity and usability of dicalcium phosphate dihydrate (DCPD) for various applications (Invited)

M. Tafu*[1]; T. Toshima[1]

1. National Institute of Technology, Toyama College, Japan

Dicalcium phosphate dihydrate (DCPD) transforms to more stable salts such as hydroxyapatite (HAp) and fluoroapatite (FAp) in an aqueous solution. This reaction has been applied hardening process of phosphate cements. In presence of fluoride ion, DCPD easily transforms to FAp. Reactivity and/or usability is important for usage of DCPD on various applications. Here we show our achievements on improvement of reactivity and usability of DCPD. We appeared that hybridization of HAp or FAp was effective for improvement on reactivity of DCPD with fluoride ion. Hybridized nano-scaled HAp or FAp acted as precursor on transform reaction of DCPD to FAp. We also appeared that particle morphology was one of the important factors on usability of DCPD powder. DCPD is generally obtained as plate-like particle. We produced petal-like DCPD particle by controlling synthesis condition and/or some additive such as acetic acid. These results demonstrate improvement of reactivity and usability of DCPD is expected to develop novel applications for DCPD.

3:20 PM

(BIO-056-2019) Additive manufacturing as the tool for the production of osteoconductive bioresorbable bone-grafting materials of complex shape (Invited)

P. Evdokimov*[1]; V. Putlayev[1]; A. Garshev[1]; E. Klimashina[1]; T. Safronova[1]; V. Dubrov[2]; I. Scherbackov[2]; N. Orlov[3]; S. Tikhonova[3]; A. Tikhonov[3]

1. Lomonosov Moscow State University, Materials Science Department/ Chemistry Department, Russian Federation
2. Lomonosov Moscow State University, Faculty of Fundamental Medicine, Russian Federation
3. Lomonosov Moscow State University, Materials Science Department, Russian Federation

Chemical, physical and mechanical compatibility of osteoconductive biomaterials for orthopaedics is a primary goal for one of the important areas of modern materials science. A bone graft material should be used as a porous active medium (scaffold), necessary for the construction of newly-formed tissue. An ideal implant should gradually dissolve and be replaced by the new bone tissue and supply inherent events for nerve and vessels regeneration during rehabilitation. The production of an implant for tissue regeneration with complex matrix framework and optimal architecture is unavoidably linked with additive manufacturing techniques. This talk tackles interdisciplinary character of the issue, being at the intersection of materials science, medicine and engineering. Touching different additive manufacturing approaches for fabrication of personalised implants for bone tissue reconstruction and the significance of interconnected pore architectonics for the guiding and the supporting function at the initial stages of osseointegration of the implant. RFBR partially supported this study under Grant No. 16-38-60203, 18-53-00034, 18-29-11079, 18-29-11070, 18-33-00789, 18-08-01473, 19-03-00940. Russian Science Foundation partially supported this study under Grant No. 17-79-20427, 18-79-00256. The authors acknowledge partial support from MSU Program of Development

3:50 PM

(BIO-057-2019) The improvement of N-doped TiO_2 photocatalyst hydrophobic composite by PTFE addition for antibacterial self-cleaning materials (Invited)

A. H. Ramelan*[1]; S. Wahyuningsih[2]

1. Sebelas Maret University, Physics, Indonesia
2. Sebelas Maret University, Chemistry, Indonesia

The conventional superhydrophobic surface offered by PTFE provides no sterilization performance and is not sufficently repellent against organic liquids as oleic acid as abundant content in food oil. These limit PTFE's application in the field of disinfection and result a lack of durability. N-doped TiO2 photocatalyst added PTFE composite material was developed to solve the self-cleaning materials both hydrophilic and hydrophobic character of dirt in surfaces. This paper reports the surface characteristics, and the bactericidal and self-cleaning performance of the newly-developed composite material built of N-doped TiO2-PTFE prepared by silane agent polydimethylsiloxane as an unity group. The material exhibited a contact angle more than 150 degrees depend on ratio of N-doped TiO2 : PTFE about 5 – 15% w/w. Compared with the N-doped TiO2 coating only, the inactivation rate of the composite material was significantly enhanced. Utilizing the N-doped TiO2 with the PTFE composite coating could successfully remove, by UV illumination, oleic acid adsorbed on its surface. These results demonstrate the potential applicability of the novel N-doped TiO2 photocatalyst hydrophobic composite material for both indoor antibacterial action and outdoor contamination prevention.

4:20 PM

(BIO-058-2019) Additive manufacturing of materials for medical diagnosis and treatment (Invited)

R. Narayan*[1]

1. North Carolina State University, USA

Photopolymerization-based materials processing approaches such as two photon polymerization may be useful for medical diagnosis and treatment. We have recently used additive manufacturing approaches to fabricate microneedle arrays for transdermal drug delivery, microneedle arrays for biosensing, scaffolds for tissue engineering, and other small-scale medical devices. Unlike conventional lithography-based fabrication and conventional subtractive fabrication methods, two photon polymerization is an additive manufacturing approach that involves spatial and temporal overlap of photons for photopolymerization within highly-localized volumes. A medical device component with an arbitrary geometry may be created by polymerizing the material along the laser trace, which is translated in three dimensions using a micropositioning system. Two photon polymerization exhibits advantages over other approaches for scalable mass production of small-scale medical devices. Several classes of inexpensive inorganic-organic hybrid materials and other photosensitive materials may be processed with two photon polymerization. In vitro cell studies and functional testing of two photon polymerization-fabricated structures will be considered. In addition, use of novel classes of photosensitive materials for medical applications will be presented.

Wednesday, July 24, 2019

B5: Nanotechnology in Medicine

Nanotechnology in Medicine

Room: York B

Session Chair: Thomas Webster, Northeastern University

8:30 AM

(BIO-059-2019) Integrated photonic-based sensors for biomedical metrology (Invited)

N. J. Castro*[2]; Z. Ahmed[1]

1. National Institute of Standards and Technology, Thermodynamic Metrology Group, Sensor Sciences Division, USA
2. NIST/University of Maryland, Joint Quantum Institute and Physical Measurements Laboratory, USA

Additive manufacturing/three-dimensional printing (AM/3DP) is a disruptive manufacturing technique which excels over traditional manufacturing technologies in speed, accuracy and efficiency. With the flexibility of incorporating various materials and functionalities within a single packaging the era of functional 3DP devices is ripe. Herein we aim to address an unmet need in the areas of tissue engineering and regenerative medicine where dynamic, real-time sensing of tissue development is absent. To that end, we are developing the use of photonic sensors to evaluate local extracellular matrix (ECM) formation and development. For the first time, real-time monitoring of de novo tissue formation will be evaluated by embedding photonic-based optical sensors within a 3D cell matrix for dynamic spatiotemporal evaluation of calcium phosphate nucleation. Notwithstanding, the current works also establishes a platform technology wherein bioresponsive photonic sensors can be integrated to monitor crucial parameters of interest (e.g. pH, temperature, strain) using standard telecom techniques leveraging economies of scale afforded by the telecom market.

9:00 AM

(BIO-060-2019) Synthesis and characterization of Quantum Dots in Therapeutic and Diagnostic Applications (Invited)

A. Nemati*[1]; E. Nemati[2]

1. Sharif University of Technology, Materials Science & engineering, Islamic Republic of Iran
2. Ecole de Technologie Superieure, Mechanical Engineering, Canada

Quantum dots (QD) have emerged as new generation of contrast agents, fluorescent labels, along with special photoelectric, photocatalytic and photoluminescence characteristics. Quantum dots advantages over traditional fluorescent dyes are their narrow emission spectra, size tunable emission wave length due to quantum confinement effect, broad absorption spectra, superior brightness and durability to photobleaching. Designing bioconjugated quantum dots to target special biomarkers, can provide simultaneous diagnostic imaging and therapy through targeted drug delivery. Another aspect is their unique photocatalytic and photoluminescence characteristics for drug delivery and many more biomedical applications. The most important factor in developing nano-carriers for biological applications is the toxicity, so recent researches have been focused on heavy metal-free formulations of QDs. In this paper we will describe two kinds of QDs. We attempt to explicate efficiencies and deficiencies of recent advances in InP/ZnS quantum dot based formulations with the least toxicity for bioimaging and therapeutic applications, as well as photocatalytic and photoluminescence characteristics of graphene quantum dots in nano-bio composites.

9:30 AM

(BIO-061-2019) Development of magnetite-gold nanoplatforms for photothermal therapy (Invited)

M. Miola*[1]; C. Multari[1]; N. Kostevsek[2]; C. Ormelli[1]; R. Gerbaldo[1]; F. Laviano[1]; E. Vernè[1]

1. Politecnico di Torino, DISAT, Italy
2. Jozef Stefan Institute, Slovenia

Nano-sized particles have been widely investigated as new therapeutic and diagnostic tool for tumor treatment. In particular, magneto-plasmonic nanoparticles, composed by iron-oxide and gold nanoparticles, have been studied for their ability to combine magnetic and plasmonic properties. This research work concerns the design of a reproducible and innovative synthesis method to synthesize magneto-plasmonic nanoplatforms with a magnetite core decorated with gold nanoparticles. Magnetite nanoparticles were synthesized by co-precipitation method, Au nanoparticles were reduced directly on magnetic nanoparticles surface by using tannic acid as reducing and capping agent. The hybrid nanoplatforms were characterized in terms of morphology, composition, magnetic response and optical properties. Both magnetic and plasmonic nanoparticles showed a pseudo-spherical morphology; hysteresis cycle measurement demonstrated the superparamagnetic behavior of magnetite nanoparticles, while UV-vis analysis confirmed the plasmonic properties of Au nanoparticles. The nanoplatforms irradiation with a laser source evidenced the materials ability to convert the received light into thermal energy useful to kill tumoral cells. Moreover, cytotoxicity tests on both healthy and cancer cells are in progress to estimate the nanoplatforms efficacy and safety.

10:20 AM

(BIO-062-2019) Say Goodbye to Hospitals and Hello to Implantable Nano Sensors (Invited)

T. J. Webster*[1]

1. Northeastern University, Chemical Engineering, USA

There is an acute shortage of organs due to disease, trauma, congenital defect, and most importantly, age related maladies. While tissue engineering (and nanotechnology) has made great strides towards improving tissue growth, infection control has been largely forgotten. Critically, as a consequence, the Centers for Disease Control have predicted more deaths from antibiotic-resistant bacteria than all cancers combined by 2050. Moreover, there has been a lack of translation to real commercial products. This talk will summarize how nanotechnology can be used to increase tissue growth and decrease implant infection without using antibiotics but using sensors (while getting regulatory approval). Our group has shown that nanofeatures, nano-modifications, nanoparticles, and most importantly, nanosensors can reduce bacterial growth without using antibiotics. This talk will summarize techniques and efforts to create nanosensors for a wide range of medical and tissue engineering applications, particularly those that have received FDA approval and are currently being implanted in humans.

10:50 AM

(BIO-063-2019) Precision Biosystems: Levitating Rare Biological Materials to 'Decode' the Fundamentals (Invited)

G. Durmus*[1]

1. Stanford University, Radiology, USA

At the convergence of engineering, biology and medicine, my research is centered on enabling solutions to real world problems at the clinical level, where traditional approaches fail. In this talk, I will present an overview of my work in the areas focused on applications of magnetic levitation and microfluidic methods for biomarker-free sorting of rare cells and rare signatures from whole blood and assembling cells in zero-gravity. Taking advantage of the unusual physics of cells in the magnetic levitation platform, we demonstrate that both eukaryotic and prokaryotic cells can be levitated and that each cell has a unique levitation profile. Furthermore, our levitation platform uniquely enables ultra-sensitive density measurements, imaging, sorting and profiling of millions of cells in seconds in real-time at single-cell resolution. This technology platform is broadly applicable to study cancer biology, as cancer diagnostics as well as drug screening in personalized medicine, tissue engineering, and bio-space research. I will present biomarker-free identification, levitational sorting of rare circulating tumor cells (CTCs) and tumor microemboli (CTM) from metastatic cancer patient blood samples. These new technologies have the broader potential to transform the way how patients are monitored, diagnosed, treated; and to create new paradigms for fundamentally understanding health and disease.

11:20 AM

(BIO-064-2019) Engineering Nanostructured Oxides on Magnesium for Biomedical Applications (Invited)

H. Liu[1]; J. Lin*[1]

1. University of California, Riverside, Bioengineering, USA

Magnesium and its alloys were considered as potential biomaterials for bioresorbable implants in recent years due to their strong mechanical properties close to natural bone and promising biological properties. However, the fast degradation of Mg in physiological fluids is the major issue that limits their broad clinical applications. To improve the corrosion resistance and enhance biological properties, e.g. biocompatibility and antimicrobial property, we have developed a layer of nanostructured magnesium oxide (MgO) onto Mg substrates through electrophoretic deposition (EPD) and anodization; both methods have been successfully used in producing uniform coatings on substrates with complex geometries and widely used in nanoparticles deposition as well as creating nanostructured surfaces. The nanostructured MgO could also provide several advantages over the conventional microstructured MgO, i.e. better bioresorbability, because of its high surface area-to-volume ratio. The developed nanostructured MgO layer was able to reduce H_2 formation as well as sustaining bone marrow derived mesenchymal stem cells (BMSC) adhesion as compared with the Mg controls, which is promising for future development of Mg-based metals for orthopedic applications. This presentation highlights the key progress on applying nanotechnology in Mg implants, which paves a way for future clinical translation of Mg-based biomaterials.

B11: Material Needs for Medical Devices

Material needs for Medical Devices II

Room: Trinity V

Session Chairs: Hideyuki Kanematsu, National Institute of Technology, Suzuka College, Japan; Srimanta Barui, Indian Institute of Science

8:30 AM

(BIO-065-2019) Oxygen defected nanoceria as highly selective biosensors (Invited)

S. Seal*[1]

1. University of Central Florida, Advanced Materials Processing and Analysis Center, USA

In recent years, numerous materials have been explored for biosensor applications. Next generation sensors are highly significant for disease diagnostics and subsequent medical therapies. Cerium oxide based nanomaterials with its regenerative catalytic abilities has gained much attention for variety of biomedical applications in recent years, especially in treating ROS (reactive oxygen species) mediated cell dysfunction. Early detection of ROS molecules is highly critical for medical diagnostics. Combining the nanoscale cerium oxide redox catalytic property with the electrochemical measurement has led to the development of biosensor platform for variety of biomolecule detection. Few examples are highlighted in detecting ROS and neurotransmitters with high selectivity and the development of enzyme free sensing platform. Some recent work from our group will highlight the development of organic electrochemical transistor (OECT) biosensors with ultra-thin nanoceria for detection of precursor molecules in the early detection of citrus greening.

9:00 AM

(BIO-066-2019) 3D inkjet printing of metallic biomaterials with strength reliability and cytocompatibility: Quantitative process strategy for Ti-6Al-4V (Invited)

S. Barui*[1]; A. Panda[1]; S. Naskar[3]; K. R[2]; S. Basu[2]; B. Basu[1]

1. Indian Institute of Science, Materials Research Center, India
2. Indian Institute of Science, Department of Mechanical Engineering, India
3. Indian Institute of Science, Centre for Biosystems Science and Engineering, India

Despite the manufacturing potential of patient-specific implants, little quantitative knowledge about the transient process physics and dynamics of 3D inkjet powder printing of biomaterials is available. We have developed a unique theoretical and experimental process strategy with a novel in situ polymerisable acrylic ink system to print Ti-6Al-4V, a metallic biomaterial. Flight dynamics of ink droplets have been captured using high speed shadowgraphy, quantifying the dimensionless numbers of fluid physics for 'printability' assessment. Washburn model was adapted to evaluate the ink infiltration time in the porous powder bed. Diffusing wave spectroscopy quantified the powder binding time during in situ polymerisation. 98.4%

interconnectivity among 10–40 μm pores with compressive modulus of 4 GPa and strength reliability (Weibull modulus ~8.1) establish the inkjet printed Ti-6Al-4V as cortical bone analogue. The unique combination of stiffness, surface roughness and wettability influence a better cell adhesion, cytoskeletal spreading, proliferation and calcium activities of murine fibroblasts on printed Ti-6Al-4V, compared to the commercial counterpart, in vitro. The quantitative understanding of the integrated process physics and dynamics to inkjet print Ti-6Al-4V can lead to a paradigm shift in commercial manufacturing of metallic implants.

9:30 AM

(BIO-067-2019) Antibiotics Loading to Hydroxyapatite/Collagen Bone-Like Nanocomposite (Invited)

M. Kikuchi*[1]; S. Oshima[1]; K. Ozeki[2]; Y. Suetsugu[1]; M. Honda[3]

1. National Institute for Materials Science (NIMS), Bioceramics Group, Japan
2. Ibaraki Unicersity, Japan
3. Meiji University, Japan

Implant associated infection become an important problem on medical and dental implants with increasing in number of surgical operation in developing countries. Medical implants in general are completely implanted into our body; thus, medical implants generally need one-time, during surgery and following short period, care. However, materials remained in human body have a potential risk to be an infection focus; therefore, biodegradable/bioresorbable bone void fillers reduce the risk. Considering the above, adsorption/desorption behavior of gentamicin sulfate (GNT), one of wide spectrum antibiotics, on hydroxyapatite/collagen bone-like nanocomposite (HAp/Col), completely substitute with new bone by bone remodeling process, were investigated. In addition, efficacy of the GNT-loaded HAp/Col was evaluated by shaking culture and inhibition zone assays using Escherichia coli (E.Coli). The HAp/Col powder having specifi surface area of 41.7±1.7 m^2/g adsorbed 3.41 mg/g of GNT and desorbed completely in 3 days after soaking in phosphate buffered saline. This period may enough to prevent initial infection because the HAp/Col starts to resorb in 5 days after implantation. The released GNT from the GNT-HAp/Col showed sufficient antibacterial effects from both assay. The GNT-HAp/Col is a good candidate for prevent initial implant associated infection.

10:20 AM

(BIO-068-2019) Biofilms formed on implanted materials and the analysis of the componenets: From the viewpoint of correlation between organic polymers and materials (Invited)

H. Kanematsu*[1]; D. M. Barry[3]; N. Hirai[2]; A. Ogawa[2]; N. Wada[1]; T. Kogo[1]; D. Kuroda[1]

1. National Institute of Technology, Suzuka College, Japan, Materials Science and Engineering, Japan
2. National Institute of Technology, Suzuka College, Chemistry and Biochemistry, Japan
3. Clarkson University, Electrical and Computer Engineering, USA

Biofilms form at the interface between solid-liquid, or solid-air-liquid interfaces by bacterial activities generally. And the bacteria existing within biofilms could have the high resistance against biocides and antibiotics. Therefore, the sensitivity and capability of implants and medical devices used at the medical fronts for biofilm formation are very important factors for the practical application. However, we already know that the biofilm formation capability differes from material to material. And we also confirmed that the biofilm components differed from materia to material, even though a certain same bacteria might form biofilms on them. However, the reason has not been enough clarified nor discussed so far. We authors classified the materials into three types, metallic materials, ceramic materials and polymers and established hypotheses for each to explain about the reason why materials could affect the biofilm contents (polysaccharides, proteins, nucleic acids or lipids). And we carried out experiments to produce biofilms on various materials in the laboratory artificially, evaluated them by Raman spectroscopy and staining. And we discussed on the relation between the biofilm formation capability and the substrate materials. In this presentation, we will show the results systemtically.

10:50 AM

(BIO-069-2019) Design, Fabrication and Performance of Multifunctional Scaffolds for Regenerating Complex Human Body Tissues (Invited)

M. Wang*[1]

1. The University of Hong Kong, Department of Mechanical Engineering, Hong Kong

Tissue engineering may provide solutions to the regeneration of "simple" tissues such as skin. There are now great needs for regenerating complex tissues such as gastrointestinal tracts. For successful tissue regeneration, scaffold-based tissue engineering is still the dominant approach. Scaffolds provide a conducive microenvironment for cells to adhere, proliferate and differentiate, leading to new tissue formation. It is also preferred now that scaffolds can induce stem cell differentiation into target tissue cells. Different nanocomposites, mainly polymer-based composites containing bioactive and biodegradable ceramic nanoparticles for hard tissue regeneration, are investigated as new tissue engineering materials. There are also a variety of scaffold fabrication techniques, e.g., freeze-drying, electrospinning and 3D printing. Multifunctionality is desirable and may be achieved for tissue engineering scaffolds. For regenerating complex tissues such as gastrointestinal tracts which have multilayered structures, through good scaffold design and by using appropriate fabrication techniques together with suitable biodegradable biomaterials, complex multifunctional scaffolds can be constructed. This lecture presents our research on multicomponent and multifunctional tissue engineering scaffolds and discusses issues in scaffold design and fabrication.

11:20 AM

(BIO-070-2019) Alpha-double-prime Ti-7.5Mo alloy for dental and orthopedic applications (Invited)

C. Ju*[1]; J. Chern Lin[1]; Y. Peng[1]; Y. Chen[2]

1. National Cheng-Kung University, Materials Science and Engineering, Taiwan
2. Joy Medical Devices Corp., Taiwan

A biocompatible, low elastic modulus Ti-7.5Mo alloy with an alpha-double-prime (α'') orthohrombic crystal structure for medical applications has been developed at National Cheng-Kung University (NCKU). The mechanical properties of this alloy can be adjusted via different processes for different applications. Its ultimate tensile strength/modulus ratio through one specific process can be more than 200% of Ti-6Al-4V ELI, 300% of grade-4 cp-Ti, and 500% of grade-2 cp-Ti, while its elongation can be adjusted to 10-40%, depending on application. The low modulus feature is expected to reduce the stress-shielding effect often observed in rigid metallic and ceramic implantation studies. This Ti-7.5Mo alloy is expected suitable for making dental crown & bridge, RPD, dental implant, orthopedic fixation, miniplate, etc. A head-to-head comparison between α'' Ti-7.5Mo and the popularly-used grade-2 cp-Ti in dental casting-related performance shows that cast Ti-7.5Mo alloy performs consistently superior to the cp-Ti. In addition to its much better castability (by 25-100%, depending on wax paten design) and machinability, the unique combination of higher strength and lower elastic modulus of Ti-7.5Mo alloy offers a far higher elastic recovery angle which has advantages over cp-Ti for certain applications such as RPD clasps. The research was funded by Ministry of Science and Technology (MOST) Grant No. 107-2221-E-006-016.

B13: Zirconia Bioceramics in Metal-free Implant Dentistry

Metal-free Implant Dentistry

Room: York A
Session Chair: Sammy Noumbissi, International Academy of Ceramic Implantology

8:30 AM

(BIO-071-2019) Zirconia Ceramic Implants versus Titanium Dental implants: What do We Know Today? (Invited)

S. Noumbissi*[1]

1. International Academy of Ceramic Implantology, USA

Modern dental implantology has used titanium and titanium alloys as the materials of choice for dental implants. After more than four decades of success, there is increasing scientific evidence that titanium implant alloys are not as stable and inert as they were once believed to be. Implanted titanium alloys used for implantation are now known and proven to be prone to corrosion attack over time and ions released in the process to induce immunological responses and other systemic health problems. Polycrystalline bioceramics such as zirconia ceramic composites thanks to their physical properties, inertness, hypoallergenicity and superior aesthetics have emerged as the materials of choice for metal free dental implantation. This presentation will present nine years of experience through a wide range of clinical cases and how metal free implants fill a long-standing void in dental implantology.

9:30 AM

(BIO-072-2019) Review on nano-technology-modified zirconia oral implants (Invited)

S. Gupta*[1]

1. International Academy of Ceramic Implantology, USA

Zirconia is gaining interest as a ceramic biomaterial for dental implant applications due to its biocompatibility and desirable mechanical properties. This presentation briefly reviews about recent nano-technology that have been applied to zirconia to improve the osseointegration of these implants. The cellular response of fibroblast, osteoblast-like cell, osteoblast cell, and epithelial cell to the modified surface is discussed in terms of their adhesion, proliferation, and metabolic activity. The presentation would also include discussion on the surface characteristics and surface roughness of different commercially available dental zirconia implants. The potential of surface nanotechnology to make zirconia a more successful dental implant material in future is highly dependent on the establishment of successful in vitro and invivo studies. Hence, further effort should be made in order to deepen the understanding of tissue response to the implant and the tissue regeneration process. The presentation concludes with future prospects of research and further challenges in developing better zirconia bioceramics and to achieve much more BIC with its counter Ti surfaces.

10:30 AM

(BIO-073-2019) One-piece vs two-piece ceramic dental implants: Current indications and clinical suggestions (Invited)

A. Borgonovo*[1]

1. University of Milan, Department of Aesthetic Dentistry, Istituto Stomatologico Italiano, Italy

In the recent years, the dental implantology has evolved towards the research of alternative materials to titanium. The zirconia implants becomes a optimal metal free alternative in modern dentistry, at first used in their one-piece variant, have been further developed thanks to the introduction of the two-piece version. In the first part of the lecture the AA describe the peculiarities of one piece zirconia dental implants and long term results of clinical and experimental studies analyzing survival and success rates, soft tissue health and radiographic marginal bone loss (MBL) with 10 -12 years follow-up. The second part of the lecture the AA present an scientific literature overview of two-piece zirconia implants, recently introduced in the panorama of ceramic implantology, offering new and different clinical solution to complete the possibility of metal free restorations, moreover the AA show their clinical experience results in order to understand current indications, morphological characteristics and success rate of these implants.

Thursday, July 25, 2019

B3: Clinical Translation of Biomaterials and Biophysical Stimulation

New Generation Biomaterials

Room: York A
Session Chairs: Surya Mallapragada, Iowa State University; Bikramjit Basu, Indian Institute of Science

8:40 AM

(BIO-074-2019) Structure/property relationships in Biomaterials at the nanoscale

F. Rosei*[1]

1. INRS, Canada

Nanostructuring materials allows to optimize their properties, by exploiting size effects. We created nanopatterns that act as surface cues, affecting cell behavior. Chemical oxidation creates nanoscale topographies, that improve biocompatibility. Our treatment provides a differential signal, selectively inhibiting fibroblast proliferation while promoting osteoblast growth in vitro. Improving antibacterial properties using laser/plasma strategies and growing graphene oxide coatings will be discussed. Finally, sensing and therapeutic approaches can be harnessed by exploiting optical properties of nanocrystals, including Quantum Dots and upconverting nanoparticles.

Electric Field Induced Tissue Regeneration and Implant Integration

Room: York A
Session Chairs: Shalini Gupta, Indian Institute of Technology Delhi; Federico Rosei, INRS

9:20 AM

(BIO-075-2019) Biomaterials Design to Control Stem Cell Fates

S. K. Mallapragada*[1]

1. Iowa State University, USA

The current gold standard for peripheral nerve repair involves autografts, which suffer from significant drawbacks such as partial denervation at the donor site. A promising alternative involves degradable conduits seeded with Schwann cells (SC) to provide physical guidance and to secrete neurotrophic factors to facilitate peripheral nerve regeneration. However, due to the difficulties in obtaining SC, we have developed graphene circuits to electrically stimulate readily-accessible bone marrow-derived mesenchymal stem cells (MSC) and transdifferentiate them to SC-like phenotypes solely with electrical stimulation. In addition, gelatin-based 3D conduits with three different microstructures as well as porous graphene foams were fabricated and the effects of conduit microstructure and mechanical properties on the transdifferentiation of MSCs into SC-like phenotypes were examined to help facilitate neuroregeneration and understand material-cell interfaces. Results indicated that certain microstructures enhanced MSC attachment, proliferation and spreading, compared to 2D-tissue culture plate counterparts. 3D-ladder-like conduit structures provided the most favorable microenvironment for MSC transdifferentiation. The synergistic combination of electrical stimulation through graphene circuits and microstructural effects through conduit design on MSC transdifferentiation to SC is being explored.

10:20 AM

(BIO-076-2019) Making a Full Circle: Advancements in Bone Grafts Based on Pure Calcium Phosphates (Invited)

V. Uskokovic*[1]

1. University of Illinois, Bioengineering, USA

There are many reasons why bone replacement materials based on pure calcium phosphates (CPs) are appealing to the clinic and the market. Their low cost, easy regulatory approvals and low risk of adverse events in vivo are only some of them. However, pure CP bone grafts have proven uncompetitive to polymeric constructs in the recent decades. Still, there are hopes that with the use of advances in materials chemistry, the composition and structure of these materials could be tailored at the nano scale to endow them with properties that typify their more compositionally complex rivals. Here I will present the work done in pursuance of this goal and demonstrate that nanoparticulate calcium phosphates could simultaneously: (a) take the form of viscous and injectable, self-setting pastes with tunable hardening kinetics; (b) yield tunable drug release profiles; (c) be naturally osteoinductive and inhibitory for osteoclastogenesis; (d) intracellularly deliver genes and other bioactive molecules; (e) accommodate an array of therapeutically active ions; (f) be processed into macroporous constructs for tissue engineering; and (g) be naturally antimicrobial, without any need for organic antibiotics. These results will be placed in the context of an ongoing effort to expand the application repertoire of calcium phosphate nanoparticles to various new biomedical applications of interest.

10:50 AM

(BIO-077-2019) Flexible Electronic Biointerfaces for Stem Cell-based Therapies (Invited)

M. Uz*[1]; M. Donta[1]; H. Greiman[1]; D. S. Sakaguchi[1]; S. K. Mallapragada[1]

1. Iowa State University, USA

Mesenchymal stem cells (MSCs), that can differentiate into specific cell lineages, hold considerable potential for cell-based tissue regeneration therapies. This study aims to develop flexible, biodegradable and implantable microcircuit interfaces that can precisely control differentiation and fate commitment of stem cell populations via electrical stimuli for neural regeneration. Our hypothesis is that the synergistic effect of electrical, physical and microstructural/mechanical cues applied via designed 3D microcircuit interfaces enables enhanced differentiation and fate commitment and consequently improved regeneration. Our rationale is that the tunable 3D microstructures provide a desirable microenvironment for cellular attachment, growth, and migration while the conductive graphene circuits enable local control of the electrical field, and when combined provide in situ, spatial and local differentiation. We have used novel microfluidics and polymer casting-based graphene transfer methods to fabricate poly (L-lactic acid)-based flexible electronic interfaces. The fabricated devices showed 3D microstructures and stable conductivities for controlling transdifferentiation of the MSCs. Our results indicated that MSCs showed significant attachment and proliferation on PLLA substrates along with ~90% of immunolabeling of Schwann cell markers (s100, s100β and p75) upon electrical stimuli-based transdifferentiation.

Cell-Material Interactions

Room: York A

Session Chairs: Miho Nakamura, Tokyo Medical and Dental University; Marta Miola, Politecnico di Torino

1:30 PM

(BIO-078-2019) Multifunctionality of piezoelectric materials towards improving cellular and antibacterial response (Invited)

A. K. Dubey*[1]

1. Indian Institute of Technology (BHU), Varanasi, Department of Ceramic Engineering, India

In recent years, a significant progress has been made towards the development of electro-active biomaterials, mimicking the electro-mechanical response of natural living bone. In this perspective, the talk will briefly cover the origin/source of the fundamental electrical responses of living bone as well as the potentiality of multifunctional ferroelectric perovskite sodium potassium niobate (NKN) as appealing electroactive alternates in orthopedics. Considering the living cells as an electrical entity, controlled and directed growth and proliferation of cells is speculated to be possible with the externally applied electrical stimulation. The talk will elaborately discuss the number of possible ways to design the electrical equivalent circuits of a living cell based on the path of ions traversed under an applied potential difference. Further, the talk will detail the various aspects of application of electric field/polarization in stimulating the growth/proliferation of cells as well as antibacterial response on ferroelectric substrates.

2:00 PM

(BIO-079-2019) Dualosome: A liposomal drug delivery platform to co-target cancer and intracellular bacteria in cancer (Invited)

R. Singh[1]; C. S. Kumar[2]; M. Banerjee[2]; S. Gupta*[1]

1. Indian Institute of Technology Delhi, Chemical Engineering, India
2. Indian Institute of Technology Delhi, School of Biological Sciences, India

Bacteria can behave both as cancer causative and cancer prevailing agents depending on their local environment. In spite of this, cancer and bacterial therapies continue to be administered discretely. We believe it is time to develop systems that not only target cancer but also clear bacteria from its niche in order to prevent secondary infections, reduce resistance and improve outcomes. We have developed a liposomal drug delivery platform called Dualosome which has the capability to co-target cancer and cancer-internalized bacteria. Dualosomes contain anticancer drug doxorubicin in the liposome core and antibacterial cationic peptide sushi S3 on the outside. Folic acid is also attached to impart specificity toward cancer cells. The efficacy of Dualosomes has been tested on S. typhi-infected Huh-7 cancer cell lines. Our results show that bacterial presence alone renders cancer therapy less effective compared to the non-infected cancer cells. The use of the copackaged system, however, is ~75% more effective in killing both cell types than either drug alone, in the encapsulated or free form. This is due to the enhanced internalization of the Dualosomes due to the positively charged sushi peptides on liposomal surface and clearing of the internal bacteria allowing anticancer drug to kill cancer cells. Animal studies are now underway to prove the clinical utility of our approach.

2:30 PM

(BIO-080-2019) 3D Graphene Foam Scaffolds for Stem Cell-based Peripheral Nerve Regeneration (Invited)

M. Uz*[1]; J. Hyung[1]; M. Donta[1]; H. Greiman[1]; A. Naclerio[2]; P. Cheng[2]; D. S. Sakaguchi[1]; P. Kidambi[2]; S. K. Mallapragada[1]

1. Iowa State University, USA
2. Vanderbilt University, USA

Mesenchymal stem cells (MSCs), isolated and derived from various connective tissue sources and transdifferentiated into Schwann cells (SCs), hold considerable potential for cell-based peripheral nerve regeneration therapies using autologous transplantation via nerve guidance conduits. In this study, Poly-L-Lactic Acid (PLLA) film with integrated graphene micro-circuits is used in combination with conductive graphene foams possessing desirable 3D microstructural/mechanical properties to provide an available cellular microenvironment for electrical transdifferentiation. Graphene-based integrated circuit designs are transferred to the PLLA film surface. Then, 3D graphene foam, prepared using chemical vapor deposition, is integrated into graphene circuits on the film surface via in situ adhesion. Our results indicated that MSCs seeded on graphene foams showed attachment, proliferation and growth within the 3D foam microstructure for 7 days with ~97% cell viability. Immunocytochemical studies indicated that ~80% of the cells showed successful transdifferentiation (labeling for SC markers s100, s100β and p75) and significantly higher amount of growth factor secretion as determined by ELISAs (NGF: ~ 2.5 pg/mL per cell) upon electrical stimuli compared to the non-transdifferentiated control MSCs. RT-PCR and Western Blot tests were used to detect the regulated genes and proteins upon electrical stimuli.

Tissue Response to Biomaterials

Room: York A

Session Chairs: Tadachika Nakayama, Nagaoka University of Technology; Palani Balaya, National University of Singapore

3:20 PM

(BIO-081-2019) Combined Vitamin and Dynamic Conditioning for Bone-Ligament Regeneration (Invited)

J. Pearson*[1]; M. Rahman[1]; G. Chiou[1]; T. Guda[1]; J. L. Ong[1]

1. University of Texas at San Antonio, USA

The enthesis between bone and ligament tissue can be affected with injury to the bone or ligament(800,000 injuries annually). Our study explores the potential for vitamins, biomaterials and dynamic conditioning for enthesis regeneration. Briefly, silk cocoons were processed to form an enthesis scaffold of silk fibroin. The bone portion was mineralized, collagen I was entangled within the ligament portion, and both were combined via aqueous methods. The scaffolds were fully characterized and seeded with human bone marrow derived mesenchymal stem cells. The scaffolds were placed in a co-culture chamber designed for tensile stimulation of the ligament. The scaffolds were examined in three environments 1)static, 2)dynamic, and 3)dynamic with ascorbic acid(ligament) and calcitriol(bone). Statistical differences were determined using One-way ANOVA for characterization and Two-way ANOVA for in vitro analysis followed by post hoc testing($p<0.05$). The dynamic vitamin group had increased ligament(scleraxis,tenomodulin) and bone(runx2,osteonectin) gene expression over the 21-day study. The static group had decreasing ligament and increasing bone expression. The dynamic silk showed increase($p<0.05$) in early ligamentogenesis(scleraxis) followed by a significant increase($p<0.05$) in late ligamentogenesis(tenomodulin) at day 21. The combination of treatments provided distinct effects with the dynamic stimulus and vitamins providing a synergistic effect and potential regenerative solution.

3:50 PM

(BIO-082-2019) Mesoporous bioactive glasses as multifunctional devices for bone regeneration

C. Pontremoli*[1]; E. Peretti[1]; A. Bari[1]; I. Izquierdo-Barba[2]; M. Vallet-Regì[2]; C. Vitale-Brovarone[1]; S. Fiorilli[1]

1. Politecnico di Torino, DISAT, Italy
2. Universidad Complutense Madrid, Spain

The treatment of bone fractures still represents a challenging clinical issue when complications due to compromised bone remodelling or bacterial infections occur. Hence, the design of a multifunctional device based on Mesoporous Bioactive Glasses (MBGs) able to stimulate bone tissue regeneration and at once inhibit bacterial adhesion represents an attractive strategy to face this challenge. MBG high surface area and tunable pore size allow the incorporation of therapeutic ions and drugs capable to impart specific biological functions such as pro-osteogenic effect. Moreover, to provide anti-adhesive properties and prevent bacteria colonization, zwitterionisation (i.e. equal number of positive and negative charges) represents a promising approach. In this work, SiO_2-CaO based MBGs containing strontium were prepared in form of nano and micro-particles and afterward loaded with drugs. The morphological and structural features and the presence of drug were investigated by FESEM, N_2 ads-des,XRD,TGA/DSC; in addition, the ability to release the cargo and the in vitro bioactivity were evaluated. MBG surface was functionalized by different routes based on silane chemistry and the successful zwitterionic functionalization was assessed by FTIR and zeta potential analysis. Biological assessment will be carried out to investigate the in vitro biocompatibility and the antibacterial capacity of the nanostructured materials.

4:10 PM

(BIO-083-2019) Electro-mechanical and polarization induced antibacterial response of 45S5 Bioglass-$Na_{0.5}K_{0.5}NbO_3$ ceramic composites

A. S. Verma*[1]; A. K. Dubey[1]; D. Kumar[1]

1. Indian Institute of Technology (BHU), Ceramic Engineering, India

Besides excellent osteoconductivity and biocompatibility of 45S5 Bioglass(BG), poor electromechanical and antibacterial properties limit its widespread clinical applications. In this context, present study investigates the effect of addition of piezoelectric $Na_{0.5}K_{0.5}NbO_3$ (NKN) on mechanical, dielectric and antibacterial behavior of BG. BG-xNKN (x=0-30vol.%) composites were prepared by solid state synthesis route at 800°C for 30min. The maximum fracture toughness (3.31±1.1MPa) and flexural strength (28.91±0.46MPa) were obtained for BG-20NKN composite. Domain switching and energy dissipation are obtained as the additional toughening mechanisms. The dielectric measurement suggested that the space charge and dipolar polarization are the dominant polarization mechanisms. Nyquist plot suggests the ionic conduction in BG-xNKN composite due to Na^+ in BG and oxygen vacancy in NKN. The E_G and E_{GB} were measured for BG-(10-30vol.%)NKN 0.597,0.934,0.945 and 0.767,0.869,1.065 eV, respectively. Irrespective of surface polarity, the polarized substrates demonstrate antibacterial response for both, gram positive (S.aureus) and gram negative (E.coli) bacteria. Surface charge generated due to poling, hydrophilicity of the sample surfaces and generation of reactive oxygen species due to microelectrolysis are obtained as the primary mechanisms for such antibacterial response.

4:30 PM

(BIO-084-2019) Electrical stimuli mediated stem cell differentiation on conducting piezopolymer for neural patch application

A. K. Panda*[1]; R. K. Krishnamurthy[1]; A. Gebrekrstos[2]; S. Bose[2]; B. Basu[1]

1. Indian Institute of Science, Materials Research Centre, India
2. Indian Institute of Science, Materials Engineering, India

Although it has been established that electromechanical stimulation plays a significant role in tissue regeneration, the behaviour of human mesenchymal stem cell (hMSc) on conducting piezopolymer is yet to be established. In the present work, Polyvinylidene difluoride (PVDF) and Multiwall carbon nanotube (MWCNT) composites have been investigated to study differentiation of hMSCs (human mesenchymal stem cell) for neural patch application. Our findings present the response of human mesenchymal stem cells (hMSCs) to the electric field stimuli (0-2 V/cm^{-1}) with an adaptation of extended neural-like morphology on piezoelectric polymeric substrates when cultured without biochemical growth factors. The fabrication technique to increase the β-phase in PVDF will be described along with quantitative phase analysis using XRD and FTIR. The commitment of stem cell towards differentiation of specific lineage corroborated with the proliferation arrest of hMScs. Immunocytochemistry using Nestin and βIII tubulin confirmed the neural differentiation of hMScs. The role of electrical stimuli and substrate conductivity on differentiation will be quantitatively described using gene expression analysis. Summarising, the presentation will be emphasized on the importance of electro-actuation on stem cell differentiation using synergistic effect of surface conductivity and piezoelectricity.

4:50 PM

(BIO-085-2019) 3D Molecularly Functionalized Cell-Free Biomimetic Scaffolds for Osteochondral Regeneration

J. Li*[1]; Q. Yao[1]; L. Wang[1]; Y. Zhu[2]; L. Li[2]

1. Nanjing First Hospital, Nanjing Medical University, Orthoaepedics, China
2. Nanjing Tech University, College of Biotechnology and Pharmaceutical Engineering, China

The construction of biomimetic scaffolds to support both cartilage and subchondral bone regeneration remains a great challenge. Herein, a novel strategy is adopted to realize the simultaneous repair of osteochondral defects by employing a self-assembling peptide hydrogel (SAPH) FEFEFKFK (F, phenylalanine; E, glutamic acid; K, lysine) to coat onto 3D-printed polycaprolactone (PCL) scaffolds. Results show that the SAPH-coated PCL scaffolds exhibit highly improved hydrophilicity and biomimetic extracellular matrix (ECM) structures compared to PCL scaffolds. In vitro experiments demonstrate that the SAPH-coated PCL scaffolds promote the proliferation and osteogenic differentiation of rabbit bone mesenchymal stem cells (rBMSCs) and maintain the chondrocyte phenotypes. Furthermore, 3% SAPH-coated PCL scaffolds significantly induce simultaneous regeneration of cartilage and subchondral bone after 8- and 12-week implantation in vivo, respectively. Mechanistically, by virtue of the enhanced deposition of ECM in SAPH-coated PCL scaffolds, SAPH with increased stiffness facilitates and remodels the microenvironment around osteochondral defects, which may favor simultaneous dual tissue regeneration. These findings indicate that the 3% SAPH provides efficient and reliable modification on PCL scaffolds and SAPH-coated PCL scaffolds appear to be a promising biomaterial for osteochondral defect repair.

5:10 PM

(BIO-086-2019) Raman and FTIR time-lapse assessment of in situ bacteria-bioceramic interactions

F. Boschetto[3]; R. M. Bock*[1]; B. J. McEntire[1]; T. Adachi[2]; E. Marin[3]; W. Zhu[4]; O. Mazda[6]; B. Bal[1]; G. Pezzotti[5]

1. SINTX Technologies, USA
2. Kyoto Prefectural University of Medicine, Department of Dental Medicine, Japan
3. Kyoto Institute of Technology, Ceramic Physics Laboratory, Japan
4. Osaka University, Department of Medical Engineering for Treatment of Bone and Joint Disorders, Japan
5. Tokyo Medical University, Department of Orthopedic Surgery, Japan
6. Kyoto Prefectural School of Medicine, Department of Immunology, Japan

Periprosthetic infections, a major contributor to orthopedic implant failure, reportedly occur at rates up to 18%. Biomaterials that inherently resist bacterial colonization are being adopted as one approach to mitigate this risk. Presently, up to 48 hour in vitro exposures of Staphylococcus epidermidis to zirconia-toughened alumina (ZTA) and silicon nitride (SN) bioceramics were conducted to explore live bacteria-biomaterial interactions by means of time-lapse Raman and Fourier Transform Infrared Spectroscopy. These data were supplemented by measurements of the nitric oxide (NO) concentration within the bacteria, fluorescence microscopy visualizations of live/dead bacteria, and pH microscopy to assess the local pH changes upon exposure of ceramic samples to an aqueous environment. Spectral features, complimented by pH microscopy, suggested bacterial environment pH shifts toward acidic values with ZTA samples. Conversely, a near-surface buffering effect whereby the local pH became more basic over time was observed in the case of SN. NO concentration was seen to intensify at the 24 hour time point for SN group, and this was followed by a precipitous drop in the presence of live bacteria. Hydrolysis of the nitride ceramic surface produces ammonia, and this phenomenon is thought to buffer the local medium and increase NO concentration within bacterial cells, inhibiting colony formation and spread.

B10: Point-of-Care Sensors and Diagnostic Devices

Point-of-Care Sensors and Diagnostic Devices

Room: York B

Session Chairs: Pankaj Kumar; Krista Carlson, University of Utah

10:00 AM

(BIO-087-2019) Rapid Diagnosis of Tuberculosis for the Point of Care Use (Invited)

M. Misra*[1]; P. Kumar[1]; S. Mohanty[2]

1. University of Nevada, Reno, Chemical and Materials Engineering, USA
2. University of Utah, Chemical Engineering, USA

Rapid disease diagnosis and continuous health monitoring are critical for addressing current global health challenges. Tuberculosis (TB) is one of the leading cause of death globally. It is crucial to detect the TB at the early stage to take early preventive majors and treatment to reduce the overall mortality. Conventional methods of TB diagnosis have challenges such as cost, diagnosis time and equipment portability. Detection of volatile organic biomarkers (VOBs), given off by mycobacterium that causes TB, present in the exhaled breath is a promising approach for TB detection and screening. In the current research, a new rapid non-invasive sensing technology has explored for TB detection at the point of care (POC) based on VOB detection. This technology utilizes a solid-state sensor based on cobalt functionalized highly ordered titania nanotubular arrays (TNAs) that interact with the VOB. The interaction of VOB with the functionalized TNAs results in a substantial change of current (orders of magnitude change) which is measured using a portable potentiostat. This technology is a simple and non-invasive diagnostic platform that can be applied to any diseases that yield volatile biomarkers.

10:30 AM

(BIO-088-2019) Highly sensitive smartphone-based cortisol detection system for real-time estimation of emotional status using Peltier module

J. Shin*[1]; S. Jung[1]; H. Jung[2]; S. Baek[1]; J. Kim[1]

1. Korea Institute of Science and Technology, Center for Electronic Materials, Republic of Korea
2. Yonsei University, Republic of Korea

Many studies reported that psychological stress is one of the main factors leading suicide and depression. In order to quantify emotional status of each subject in real time, we have newly developed a self-stress diagnostics kit, also named as the Smart Stress Phone, which consists of a lateral flow immunosensor, origami smartphone holder, portable incubator, and smartphone-based colorimetric analysis system. Since salivary cortisol is known as a psychological stress biomarker, a concentration of salivary cortisol from 9 subjects was measured using the Smart Stress Phone in the morning (8:00 AM) and afternoon (4:00 PM). Since the concentration of cortisol needed to be measured from 1.0 ng/mL to 10.0 ng/mL, we have employed colorimetric detection system for the stress diagnostics kit (Limit of detection: 1.0 ng/mL). Thanks to keeping temperature at 34 °C using the incubator based on Peltier modules, the sensor sensitivity was enhanced due to fully activated conjugation between antibodies and antigen. In addition, we successfully validated an accuracy of the device by comparing the salivary cortisol using commercialized ELISA kit and the results from our device ($p < 0.05$). Thus, we expect that the Smart Stress Phone can be a powerful tool for the patients, who suffer from psychological stress, to estimate emotional status in real time in the near future.

10:50 AM

(BIO-089-2019) Engineered Nanostructured Materials for Electrochemical Detection of Volatile Organic Compounds Associated with Pathological Conditions (Invited)

C. Willis[1]; A. Tripathy[3]; Y. Saffary[1]; L. McKinnon[1]; M. Misra[2]; S. Mohanty*[1]

1. University of Utah, Chemical Engineering, USA
2. University of Nevada, Reno, Chemical and Materials Engineering, USA
3. University of Utah, Bioengineering, USA

VOCs are a diverse group of molecular compounds that are volatile or semi-volatile at room temperature. Many of these VOCs are associated with pathological conditions such as pneumonia, tuberculosis, and colorectal cancer. The compounds are found in various fluids such as urine, sweat and breath. These VOCs present a unique opportunity for non-invasive testing of disease because they act as unique biomarkers for these disease states. However, in order to analyze such compounds, advanced analytical methods such as gas chromatography/mass spectrometry are used. While this is a very powerful technique, it is not practical for use in health care settings. There is a significant need for portable sensing technology that can be used at the point-of-care to empower patients and healthcare providers to manage disease. This presentation will focus on portable electrochemical methods that utilize a variety of engineered titania nanostructured sensing substrates, and engineered electroactive solutions for detection of various VOCs that are related to pneumonia, colorectal cancer, and tuberculosis. Several electrochemical analytical methods will be presented illustrating the advantages and disadvantages of each approach for a given VOC. These methods illustrate the potential of rapid detection of disease at the point-of-care.

11:20 AM

(BIO-090-2019) Detection of Alcohol using One Dimensional Nano-structured Titania

A. Ralls*[1]; P. Kumar[2]; P. Menezes[1]; M. Misra[2]

1. University of Nevada, Reno, Mechanical Engineering, USA
2. University of Nevada, Reno, Materials and Chemical Engineering, USA

Semiconducting materials can be applied to a multitude of applications including but not limited to: supercapacitors, transistors, solar cells and sensors. Given the vast array of existing semiconducting materials, metal oxides particularly stand out as they are cost efficient. Designing the metal oxide at nanostructure level can facilitate use of these materials for chemical sensor application. Large surface area due nanostructure design create an efficient sensor by providing increased opportunity for materials and analytes interaction. One material that has gained much traction in recent years is titanium dioxide (TiO_2). The reason being can be attributed to the band gap that this material has allowing for a minimal loss of electrons as well as its impressive corrosion resistant properties and high-temperature stability. Because of these impressive properties, TiO_2 proves to be an optimal material for chemical sensing applications. In this research, we demonstrate the use of nanostructured TiO_2 (NT) for the detection of Alcohol in ppb level. A particular focus will be on determining the validity, selectivity, and sensitivity of the NT sensor for alcohol detection. A detailed mechanism of alcohol detection will be presented.

B11: Material Needs for Medical Devices

Material needs for Medical Devices III

Room: Trinity V
Session Chairs: Biqiong Chen, Queen's University Belfast; Min Wang, The University of Hong Kong

8:30 AM

(BIO-091-2019) Isolation of Circulating Tumor Cells from Clinical Blood Samples by Charged Nanoparticles (Invited)

D. Shi*[1]; Y. Wang[2]

1. University of Cincinnati, Mechanical and Materials Engineering, USA
2. Tongji University School of Medicine, Shanghai East Hospital, China

A major challenge in early cancer diagnosis is isolation of circulating tumor cells (CTCs) from clinical blood samples. The current CTC detection technologies include microfluidic isolation and immunomagnetically labeled cell detection. In this presentation, a new CTC isolation strategy will be reviewed based on the surface-charged, superparamagnetic nanoparticles capable of binding on CTC surfaces for magnetic separation from clinical samples. The detection mechanism will be identified in terms of cancer metabolism and bio-electrical manifestation of the Warburg effect. The perpetuating secretion of a large amount of lactate acid inevitably produces a net of negative charges on the cancer cell surfaces. By rendering the magnetic nanoparticles positively charged via surface functionalization, they can strongly bind onto the negatively charged cancer cells enabling subsequent magnetic separation. We present recent results on CTC isolation from both mimetic and clinical blood samples, which show a high CTC detection sensitivity, even in the original concentration of 10 cells per mL mimetic blood sample. The circulating tumor cells in the peripheral blood of cancer patients can be well identified by cellular morphology and immunofluorescence staining.

9:00 AM

(BIO-092-2019) Cell Fiber-incorporated Electrospun Nanofibrous Scaffolds for Tendon/Ligament Regeneration (Invited)

H. Sun[1]; H. Li[1]; Y. Xu[1]; M. Wang*[1]

1. The University of Hong Kong, Department of Mechanical Engineering, Hong Kong

Nanofibrous scaffolds, which can be conveniently made by electrospinning, are much favored for regenerating human body tissues as they resemble the nanofibrous extracellular matrix (ECM) of native tissues. But cell migration in electrospun scaffolds is hindered due to small pore sizes. Embedding cell-laden fibers in the scaffolds can solve the problem. Growth factors (GFs) play important roles in tissue formation and electrospun scaffolds are effective GF-delivery vehicles. Mesenchymal stem cells (MSCs) are increasingly used in tissue engineering since MSCs can differentiate into targeted types of cells. Among different GFs, basic fibroblast growth factor (bFGF) upregulates gene expression of tendon/ligament specific ECM proteins and facilitates the proliferation and differentiation of MSCs toward fibroblasts. In this study, scaffolds consisting of cell fibers with bone marrow-derived MSCs and bFGF-encapsulated nanofibers were fabricated. PLGA was employed to form bFGF-containing fibers, and cell fibers were made from Na-alginate solutions. The structure, bFGF release and biological performance of scaffolds were studied. MSCs exhibited high viability and proliferated well in in vitro experiments. A steady and sustained release of bFGF was observed. MSCs in scaffolds encapsulated with bFGF proliferated faster than in the control group, showing the effect of local bFGF delivery.

9:30 AM

(BIO-093-2019) Tough double network nanocomposite hydrogels for potential soft tissue reconstruction (Invited)

B. Chen*[1]

1. Queen's University Belfast, United Kingdom

Conventional hydrogels are often weak, limiting their application in the repair and reconstruction of load-bearing soft tissues. Various efforts have been made to improve the mechanical properties of hydrogels, including double network hydrogels and nanocomposite hydrogels. In this work, a series of double network nanocomposite hydrogels, based on biocompatible polymers and natural montmorillonite clay, were prepared and investigated. By manipulating the chemical composition and reaction condition, it is possible to obtain double network nanocomposite hydrogels with controlled swelling behaviour, high toughness and excellent resilience. Some of these hydrogels also show other interesting functionalities such as UV protection, pH sensitivity and or solvent sensitivity. The hydrogels may be manufactured into various shapes and forms including microfibers, facilitating their potential use in soft tissue repair and reconstruction as well as other aquatic applications.

10:20 AM

(BIO-094-2019) Personalized Wearable Metabolic Rate Monitors (Invited)

P. Gouma*[1]

1. The Ohio State University, MSE, USA

There is a need for technological breakthroughs that lead to easy-to-use, cheap, non- invasive and robust devices capable of instantaneously calculate metabolic rates and body functions, such as fat burning over muscle. Methods designed for monitoring fatty acids metabolism aim to detect Ketone bodies (β-hydroxybutyrate, acetoacetate and acetone) which are produced by the oxidation of fatty acids (metabolism) in the liver when glucose is not readily available. Accordingly, the concentration of Ketone bodies in human systems (and animals) can directly indicate the metabolism rate of fatty acids. Ketone bodies can be detected in exhaled breath and skin released gas. Acetone has been shown to be exhaled with breath and to be emitted through skin gas from accessible skin areas (e.g., hands, arms, fingers), which enables easy, non-invasive and continuous collection of acetone samples. Also, it has been established that there is a direct correlation between acetone released from skin and acetone exhaled with breath, which, in turn, has a direct correlation to acetone content in blood. Accordingly, by measuring the concentration of skin emitted acetone, we can monitor the burning of fatty acids. This work describes wearable metabolic rate monitors developed by our group that aim to provide the individual with useful feedback on behavioral modifications towards improving health and weight control.

10:50 AM

(BIO-095-2019) Biomimetic Calcium Phosphorous Titania Nanotubes for an Efficient Biofunctional Implant (Invited)

T. Shokuhfar*[1]

1. UIC, USA

The modification of surface features such as nano-morphology/topography and chemistry have been employed in the attempt to design titanium oxide surfaces able to overcome the current dental implants failures. The main goal of this study is the synthesis of bone-like structured titanium dioxide (TiO_2) nanotubes enriched with Calcium (Ca) and Phosphorous (P) able to enhance osteoblastic cell functions and, simultaneously, display an improved corrosion behavior. To achieve the main goal, TiO_2 nanotubes were synthetized and doped with Ca and P by means of a novel methodology which relied, firstly, on the synthesis of TiO_2 nanotubes by anodization of titanium in an organic electrolyte followed by reverse polarization and/or anodization, in an aqueous electrolyte. The chemical analysis of such nanotubes confirmed the presence of $CaCO_3$, $Ca_3(PO_4)_2$, $CaHPO_4$ and CaO compounds. The nanotube surfaces submitted to reverse polarization, presented an improved cell adhesion and proliferation compared to smooth titanium. Furthermore, these surfaces displayed a significantly lower passive current in artificial saliva, and so, potential to minimize their bio-degradation through corrosion processes. This study addresses a very simple and promising multidisciplinary approach bringing new insights for the development of novel methodologies to improve the outcome of osseointegrated implants.

Material needs for Medical Devices IV

Room: Trinity V

Session Chairs: Chien-Ping Ju, National Cheng-Kung University; Jiin-Huey Chern Lin

1:30 PM

(BIO-096-2019) Antimicrobial-releasing Mesoporous Multimaterials for Load-bearing Implant Applications (Invited)

A. Braem*[2]; C. D'Haeyer[2]; K. Thevissen[1]

1. KULeuven, Centre for Microbial and Plant Genetics, Belgium
2. KU Leuven, Dept. of Materials Engineering, Belgium

The current trend towards rough surfaces for load-bearing bone implants allows achieving successful osseointegration but also entails a high risk for bacterial colonization and subsequent development of biofilm associated infections. Implants incorporating and locally releasing antimicrobial molecules at their surface in a controlled manner are proposed as a possible anti-infective strategy. Mesoporous bioceramics, e.g. silica or bioactive glass, are of interest as these materials exhibit tunable pore structures allowing adjusting the diffusion kinetics, and hence the release profile, of molecules through their pores. However, when used as coatings, these materials are fragile and cannot be refilled leading to a premature depletion of the drugs. As an alternative, we have integrated these mesoporous carriers into a high-strength metal matrix thereby establishing an effective diffusion barrier within the bulk of the implant material. This allowed realizing a constant and continuous release of therapeutic concentrations of chlorhexidine, an antimicrobial agent commonly applied in mouthwashes, from an internal reservoir to the implant surface. The released chlorhexidine remained effective in the prevention and eradication of biofilm formation of various pathogens. Overall, the results show that such multimaterial implant systems can take metal-based drug eluting systems to a clinical level.

2:00 PM

(BIO-097-2019) A fast-healing calcium-based bone substitute material jointly developed by National Cheng-Kung University and Joy Medical Devices Corporation (Invited)

J. Chern Lin*[1]; C. Ju[1]; J. Lee[2]; P. Lin[2]; C. Hsu[3]; B. Yang[4]

1. National Cheng-Kung University, Materials Science and Engineering, Taiwan
2. National Cheng-Kung University Medical College and Hospital, Surgery, Taiwan
3. National Cheng-Kung University Hospital, Orthopedics, Taiwan
4. Joy Medical Devices Corp., Taiwan

A series of synthetic, inorganic, highly osteoconductive and fully resorbable calcium-based bone substitute materials have been developed by a joint research project of National Cheng-Kung University and Joy Medical Devices Corporation of Taiwan. The granular type material is a highly porous product characterized by its high resorption rate and fast healing capability, while the cement type product is featured by its non-dispersive behavior in blood/body fluid. The safety and efficacy of these materials are confirmed by a series of chemical/physical characterization and biocompatibility tests. The animal models for implantation tests include SD rat femur body, New Zealand white rabbit femur condyle and mandible, Lanyu pig mandible and osteoporotic goat spine. Histopathologic examination indicates that the implants of both types are always intimately integrated with surrounding bone substantially without foreign body or other undesirable tissue reactions. The granular implant is fast replaced by new bone with an early-stage new bone formation rate significantly higher than the autologous group. Clinical case reports using these products include sinus lift, ridge augmentation, frontal bone augmentation and treatment for various types of fractures. The research was funded by Southern Taiwan Medical Device Industry Cluster (CY-05-08-38-107).

2:30 PM

(BIO-098-2019) 3D-printing of Bioceramics for Bone Regeneration Applications (Invited)

R. Gadow*[1]; S. Esslinger[1]; A. Bernstein[2]

1. Institute for Manufacturing Technologies of Ceramic Components and Composites, University of Stuttgart, Germany
2. Musculoscelletal Research Lab, Germany

The use of bioceramics like calcium phosphates or bioactive glasses for the regeneration of critical bone defects, as they can occur for example after serious injuries or diseases is under intensive research worldwide. Additive manufacturing technology make it possible to process these ceramics into customized patient-specific implants, so called scaffolds. In most cases resorbable temporary prosthetic devices are required in contrast to bioinert permanent implants. The latter ones feature dense structures with high strength. In this work the process chain of powder-based inkjet-3D-printing of bioceramic devices is presented. This includes the technology of bioceramic suspensions from bioglass, calcium phosphates and composites and spray dry granulation to obtain granulates with suitable flowabilty. 3D-printing is performed from CAD-modeling to post-processing of the printed structures. Printed components are sintered and characterized with respect to mechanical properties and in vitro biocompatibility. After sintering the scaffolds show high porosity (about 70 %) and high surface roughness (Ra about 25 μm, Rz up to 200 μm) which is beneficial for the colonization by bone cells. The compressive strength was lower than 1 MPa for every scaffolds. In vitro tests using MG-63 cells showed the suitable growth of cells on the outer and inner surface of the scaffolds and the formation of hydroxyapatite crystals.

3:20 PM

(BIO-099-2019) Scalably-nanomanufactured atomically-thin chiral semiconductor for human-integrated ubiquitous electronics and smart sensors (Invited)

W. Wu*[1]

1. Purdue University, School of Industrial Engineering; Birck Nanotechnology Center; Regenstrief Center for Healthcare Engineering, USA

The reliable production of atomically-thin crystals is essential for exploring new science and implementing novel technologies in the 2D limit. However, ongoing efforts are limited by the vague potential in scaling-up, restrictions on growth substrates and conditions, small sizes and/or instability of synthesized materials. I will discuss our recent progress in the fabrication of large-area, high-quality 2D chiral semiconductor, tellurene, by a substrate-free solution process. The tellurene crystals exhibit process-tunable thicknesses from a monolayer to tens of nanometers, and lateral sizes ~ 100 um. Our prototypical tellurene transistor device, which is air-stable, shows an excellent all-around figure of merits compared to existing 2D materials. We further carry out the first experimental exploration of piezotronic effect in tellurene and systematically investigate the piezotronic transport properties. The coupling between the piezoelectric and semiconductor properties in such chiral material system enables the design and implementation of novel electronic devices and smart sensors that can interact with the mechanical stimuli. Our approach has the potential to produce high-quality, ultrathin functional materials with good control of composition, structure, and dimensions for human-integrated electronics, wearable devices, and smart sensors.

3:50 PM

(BIO-100-2019) Suspension Flame Sprayed Metal Doped Calcium Phosphate Coatings with Antibacterial Properties for Infection Prophylaxis (Invited)

R. Gadow*[1]; A. Killinger[1]; P. Krieg[1]; A. Bernstein[2]

1. Institute for Manufacturing Technologies of Ceramic Components and Composites, University of Stuttgart, Germany
2. University Hospital of Freiburg, Musculoscelletal Research Lab, Germany

High Velocity Suspension Flame Spraying (HVSFS) has been successfully employed to produce a wide variety of bioceramic coatings for prosthetic devices and bone implants. The HVSFS process has proven to be capable to process biomaterials resulting in dense and well adherent coatings on various types of metal and ceramic substrates. Degradable bioceramic coatings offer a faster osseointegration of endoprosthetic structures. A common problem that occurs after the application of all types of implants is the risk of infection due to the presence of bacteria which can result in severe post operative inflammation reactions associated with a high risk of losing the implant. In a novel approach, metals with known antibacterial properties are incorporated into the coating as a nanosize dispersion dopant to reduce the risk of inflammation. Metal doped coatings based on bioceramics were suspension flame sprayed using modified suspensions containing additional metals or metal salt based precursors. These coatings were evaluated regarding their microstructure and phase composition, as well as their in-vitro behavior. The presence of metal and metal oxide particles in the coating were characterized using micro-Raman and SEM. To evaluate the biocompatibility, a live/dead-assay study based on MG-63 cells was performed. Results showed no evidence for any cytotoxic reaction

4:20 PM

(BIO-101-2019) Design of Biomaterials by Simulation and Experiment: Molecular Recognition, Assembly, and Applications (Invited)

H. Heinz*[1]

1. University of Colorado-Boulder, USA

The development of biomedical materials continues to involve extensive trial-and-error studies while rational understanding and design using modeling and simulation play an increasing role thanks to more accurate models and affordable computing resources. Strong support in the development of biomaterials and quantitative property predictions at the 1 to 1000 nm scale are feasible using the Interface force field (IFF) to understand recognition and assembly of metal, oxide, and biomineral nanostructures for various applications. We will discuss different mineral surfaces and interactions with organic compounds, implications on nanocrystal growth and morphology, as well as rules of molecular recognition and self-assembly derived from simulations. Specific adsorption and assembly of peptides and macromolecules on metallic and oxide/hydroxide nanostructures will be described according to measurements and simulations, including predictions in chemical accuracy and guidance in designing new commercial products. Applications to low dimensional materials, catalysts, hydrogels, and therapeutics will be discussed. The realistic representation of polar chemical bonding, specific surface chemistry, and electrolyte composition in models supports accurate reactive simulations up to the large nanometer scale with heuristic inputs from quantum mechanics and experiment.

4:50 PM

(BIO-102-2019) Better Osteogenesis of Electrically Active Hydroxyapatite-Calcium Titanate Biocomposites in a Rabbit Animal Model (Invited)

P. K. Mallik[1]; K. Balani*[2]; B. Basu[3]

1. Indira Gandi Institute of Technology Sarang, Metallurgical and Materials Engineering, India
2. IITKanpur, Materials Science and Engineering, India
3. IISc Bangalore, Materials Research Centre, India

HA is a highly biocompatible and bioactive materials used for variety of biomedical applications. However, HA has very poor electrical conductivity and inherent brittleness. Recently, $CaTiO_3$ has been approved due to its better biocompatibility and bioactive material compared to HA. In the present study, to determine the temperature (RT-200°C) and frequency (100Hz-1MHz) dependent electrical conductivity properties of a HA-$CaTiO_3$ composites and their effect on osteogenesis with living tissue using rabbit animal model. Subsequently, biocompatibility and its percentage neobone formation were estimated in vivo using histological and histomorphometrical analysis. As result, compared with pure HA as a control, HA-80 wt% CT improved the biocompatibility and tissue integration. The important result is that the AC conductivity of HA-80 wt. % $CaTiO_3$ composites was measured $10^{-5}\Omega^{-1}$ cm^{-1} at 1MHz frequency and temperature below 200°C. In addition, results suggest that by the addition of $CaTiO_3$, better the tissue integration were observed after 12 weeks of implantation in rabbit. The relative percentage of new bone formation of HA-80 wt% CT composite was 125%, while assuming control as 100%. Finally, HA-80%CT posses enhanced biocompatibility and osteointegration compared to HA by addition of $CaTiO_3$, thereby improving its potential for clinical application.

Friday, July 26, 2019

B6: Advance Materials and Devices for the Treatment of Brain Disorders

Advanced Materials and Devices for the Treatment of Brain Disorders

Room: Trinity IV
Session Chair: Tolou Shokuhfar, University of Illinois at Chicago

8:30 AM

(BIO-103-2019) Novel Method in the Treatment of Cerebrospinal Fluid (CSF) Leaks (Invited)

T. Shokuhfar[1]; M. McClendon[1]; S. Ansari[1]; S. Stupp[1]; A. Shaibani*[1]

1. Northwestern University, USA

Purpose: CSF leaks whether iatrogenic, post-traumatic or spontaneous are increasingly recognized and are a significant cause of headaches, post-procedural morbidity, and patient discomfort. Serious leaks are usually treated with an epidural injection of either autologous blood or other materials, such as fibrin glue. Fibrin glue is extremely difficult to inject through needle-based procedures as it is designed for use in an open surgical setting. The purpose of this study is to evaluate the safety and effectiveness of polyamide nanofibers in contact with the CSF in vitro. Method: This study includes 10 CSF samples from adult patients who need lumbar puncture as part of their standard of care. Results: Successful gelation of all polyamide nanofibers in contact with CSF. Conclusion: Polyamide nanofibers are fully liquid at room temperature but undergo gelation when exposed to ionic materials like CSF which could be used for the treatment of CSF leaks.

9:00 AM

(BIO-104-2019) Iron oxide Cage Protein Nanoparticles for Applications in Treatment of Brain Tumor (Invited)

T. Shokuhfar*[1]; R. Shahbazian Yassar[1]

1. UIC, USA

The advent of nanotechnology in medicine (Nanomedicine) has offered the development of promising new weapons against various cancers, including malignant brain tumors. Metal oxide nanoparticles (NPs) such as iron oxide exhibit many properties which enhance their suitability as therapeutic agents. A wide variety of NPs have been created, with ingenious strategies for binding and destroying cancer cells, including glioblastoma and medulloblastoma. Here we investigate a biological NP with an iron oxide core (Ferritin protein) as potential biomimetic and patient specific NP for treatment of brain tumor. We present how Ferritin Iron Oxide NPs can be used to resolve critical issues such as NP delivery into brain tissue (across the blood-brain barrier (BBB) or by convection-enhanced delivery), toxicity, and binding to tumor cells. This protein/metaloxide NP can potentially bypass intact BBB by being transported across it by means of adsorptive-mediated transcytosis. Since Ferritin can be collected from the patients own sample (blood, tissue, etc.)This study can introduce a new realm for patient specific and nontoxic treatment of brain tumors.

9:30 AM

(BIO-105-2019) Dual hybrid approach for HDPE/ UHMWPE nanocomposites towards improved strength and cytocompatibility for orthopedic applications

S. A. Bhusari[1]; V. Sharma*[1]; S. Bose[2]; B. Basu[1]

1. Indian Institute of Science, Material Research Centre, India
2. Indian Institute of Science, Materials Engineering, India

The present study demonstrates the efficacy of 'dual' hybrid approach for an optimized HU (60% HDPE-40% UHMWPE) blend reinforced with nanofiller for hip acetabular socket applications. In particular, a unique synthesis strategy will be described for better dispersion of surface functionalized Graphene Oxide (mGO) in PE matrix. Melt-extrusion together with injection molding of HU blend with different proportions (≤ 3 wt.%) of mGO was conducted to fabricate nanocomposites. The uniform dispersion of mGO, confirmed using X-ray micro computed tomography and transmission electron microscopy, facilitated effective interfacial adhesion and compatibility with polymer matrix. The varying mechanical properties and cell viability with GO/mGO addition to PE blend will be critically discussed in reference to the structural modification of GO, crystallinity and nature of dispersion of fillers. The nanocomposites with 1 wt.% mGO resulted in an increased ultimate tensile strength by 120% (upto 65 MPa), when compared with neat blend. Moreover, the nanocomposites supported good C2C12 murine myoblast cell attachment and proliferation, in vitro, in statistically insignificant manner with respect to matrix. Considering the experimental results, the potential of HDPE/UHMWPE nanocomposite for bone tissue engineering applications will be emphasized in the presentation.

9:50 AM

(BIO-106-2019) TAT Functionalized Liposomes as Drug Carriers for the Treatment of Brain Infection Diseases

C. Bartomeu Garcia*[1]; T. Webster[2]; D. Shi[1]

1. Northeastern University, Chemical Engineering, USA
2. Northeastern University, USA

Among all brain inflammatory diseases, bacterial meningitis is one of the most aggressive infections that without the adequate treatment, can lead to death. Moreover, the 20 percent of the population that suffer this disease and manage to survive end up with permanent disabilities and brain damage. The emergence of drug resistant bacteria has increased the difficulty for the treatment of this disease. These bacteria are not susceptible to any of the current antibiotics,

which kill the non-resistant bacteria promoting the propagation of drug resistant bacteria and the formation of biofilms. To this end, we developed an alternative drug delivery system to fight brain infections and overcome bacteria drug resistance. Fusogenic liposomes, also known as pH-sensitive liposomes, were reported as drug carriers, to target and promote the release of the antibiotic directly inside the bacteria cells. Liposomes were functionalized with a cell penetrating peptide TAT (47-57) to increase their permeability through the Blood Brain Barrier (BBB). This cell penetrating peptide has shown good permeability through the BBB in previous research, making it a crucial component of our liposome system. Liposomes were prepared by lipid film rehydration and functionalized with the cell penetrating peptide TAT (47-57) using wet chemistry. They were characterized by transmission electron microscopy, loaded with different antibiotics and tested against the bacteria commonly associated with bacterial meningitis, Streptococcus pneumoniae, methicillin-resistant Staphylococcus aureus (MRSA), and Escherichia coli. Results showed excellent antibacterial activity against S. pneumoniae and MRSA, demonstrating their ability to kill antibiotic resistant bacteria. These particles were also tested against astrocytes and endothelial cells, main cells that form the BBB, showing no cytotoxicity effects and reducing the antibiotic cytotoxicity against these cells. Finally, static BBB studies showed promising results about the ability of these liposomes to cross this tissue barrier and fight the bacteria located at the brain. Providing evidence that this liposomal system can be a safe, alternative means for treating bacterial meningitis.

10:10 AM

(BIO-107-2019) In situ Liquid Cell-TEM Studies of Iron-Oxide Biomineralization in Bacteria and Proteins (Invited)

E. Firlar[1]; R. S. Yassar[2]; S. Narayanan[1]; T. Shokuhfar*[1]

1. University of Illinois at Chicago, Bioengineering, USA
2. University of Illinois, Department of Mechanical and Industrial Engineering, USA

Investigation of in situ biomineralization has become prevalent because of the necessity to synthesize these minerals on the bench for today's needs. Understanding how these minerals nucleate and grow using electron microscopes at nano-scale has been a great challenge due to (i) the need for keeping cells and bacteria live for in situ biomineralization; and (ii) the need for keeping proteins non-degraded. Liquid cell electron microscopy was devised to monitor activities in living organisms or in liquid media due to the need to overcome the evaporation of the liquid components in the electron microscope. Graphene liquid cell, a recently developed type of liquid cell electron microscopy, enables monitoring structures encapsulated between two monolayers of graphene. In this work, we demonstrated via graphene liquid cell transmission electron microscopy that bacteria could be kept alive during electron imaging by showing intracellular biomineralization activity. Furthermore, via the same technique, ferritin proteins from both human heart and human spleen were compared with respect to their crystal structure and chemistry, which will help understanding of effect of light and heavy subunits in ferritin on the iron oxide core formation. Comprehension of live nano-scale events via this technique will open new doors for understanding of other marvels in living biological species or proteins.

B11: Material Needs for Medical Devices

Material needs for Medical Devices V

Room: Trinity V

Session Chairs: Dirk Ortgies, Instituto Ramón y Cajal de Investigación Sanitaria IRYCIS; Andrew Thom, Medtronic; Yusuf Khan, University of Connecticut Health Center

8:30 AM

(BIO-108-2019) Fabrication and Characterization of Photo-crosslinked Alginate based paste for Orthopaedic application (Invited)

K. Maji*[1]

1. National Institute of Technology (NIT), India

Introduction: Operative reconstruction of bone defects beyond a certain size is mandatory and still remains a challenge to trauma and orthopedic surgeons. Our objective is to develop an injectable as well as photocurbale artificial bone substitute material comprising of biopolymer functionalized hydroxyapatite nanoparticles embedded in photcurbale alginate based matrix. Method: In situ synthesis of surface thiol-functionalized Hydroxyapatite would be carried out by co-precipitation of Si doped HAp. Methacrylated alginate was synthesized by adding required amount of methacrylic anhydride into alginate soluiton at pH 8. Methacrylated alginate and required amount of surface functionalized HAp nanoparticles would be stirring to obtain a stable suspension. Photoinitiator Irgacure-2959 solution with controlled concentration will be added to alginate solution and the solution will be poured in a mould placed at the centre of a UV oven for short time. Results: The prepared paste exhibited low cytotoxicity when cultured with Meschenchymal stem cell. MSC's are remained metabolically active in Live/Dead cell staining and MTT assay. Moreover, the influence of BMP2 (growth factor) on cell viability and proliferation during was examined in alginate paste. Conclusion: These findings support the use of photo-cross-linked alginate hydrogels as biomaterial scaffolds for Orthopaedic application.

9:00 AM

(BIO-109-2019) Luminescent nanomaterials for in vivo bioimaging in the frequency and time domain (Invited)

D. H. Ortgies*[1]; M. Tan[2]; E. Ximendes[3]; J. Hu[4]; B. del Rosal[4]; E. Martín Rodríguez[5]; C. Jacinto[3]; N. Fernandez[6]; G. Chen[2]; D. Jaque[4]

1. Instituto Ramón y Cajal de Investigación Sanitaria IRYCIS, Spain
2. Harbin Institute of Technology, School of Chemistry and Chemical Engineering, China
3. Universidade Federal de Alagoas, Instituto de Física, Brazil
4. Universidad Autónoma de Madrid, Departamento de Física de Materiales, Spain
5. Universidad Autonoma de Madrid, Departamento de Física Aplicada, Spain
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Advancements in nanotechnology together with ever cheaper infrared cameras have brought forward the possibility of optical whole-body imaging. Working in regions of the electromagnetic spectrum in the near infrared defined as biological windows (NIR-I: 680 – 950 nm, NIR-II: 1000 – 1450 nm) allows researchers in biomedicine to look under the skin or through a small animal. Nevertheless new challenges have risen especially the predominance of autofluorescence of biological tissues (for example due to melanin), which hamper the application of classical fluorescent biomarkers most comonly organic dyes. We present two strategies to avoid this problem by employing firstly luminescent nanomaterials whose frequency lies in the NIR-II and secondly by applying nanoparticles whose fluorescence lifetimes are orders of magnitudes longer than those of the compounds responsible for tissue autofluorescence. By further developing the latter approach with a careful choice of biocompatible materials, a device for time-gated multiplexed in vivo imaging was designed, constituted by an infrared camera and a simple pulsed laser-diode that are connected through a time delay circuit. Employing nanoparticles with different lifetimes (0.1 – 1.5 ms) allowed therefore a signal analysis in the time domain and the remote visual differentiation of overlaping organs in an in vivo mouse model.

9:30 AM

(BIO-110-2019) New Materials for High Reliability Feedthroughs for Implantable Medical Devices (Invited)

A. Thom*[1]; B. Tischendorf[1]

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Medtronic has been using a patented Lanthanum Borate (LaBor) glass [US 8,288,654] as the insulating material in ultra-high reliability feedthroughs for several years. This work investigated the effect of adding alumina to the LaBor glass to tailor its material properties for different pin materials. Finite element analysis (FEA) showed that coefficient of thermal expansion (CTE) of the sealing glass is the dominant material property affecting residual stress state of the glass seal. The analysis identified alumina as a promising additive for the glass. Bulk shapes were fabricated for measuring material properties. Functional feedthroughs were made and subjected to accelerated life testing (ALT) to estimate the long-term biostability at 37°C. The measured CTE and Young's modulus of the modified glass are reasonably predicted by literature descriptions for lower and upper bounds. The modified glass showed good resistance to crack growth due to pin manipulation, consistent with the increase in measured fracture toughness. There was no difference in the kinetics of corrosion layer growth between the pure glass and modified glass. Excellent biostability of the modified glass is predicted at 37°C for device lifetimes which are expected to exceed 10 years. These results indicate that the alumina loaded LaBor glass is well suited for use in ultra-reliable feedthroughs in implantable medical devices.

10:00 AM

(BIO-111-2019) Synthesis of customized bioceramic based scaffolds for bone tissue engineering by selective laser melting (Invited)

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2. Instituto de Cerámica y Vidrio, CSIC C/Kelsen, Spain

The repair and regeneration of load-bearing defects by bioceramic scaffolds remain a significant clinical challenge resulting from disease or trauma. The needs for repair and regeneration are one of the key assets for the synthesis of the scaffolds for load-bearing repair applications. The criteria include (1) porous structure, (2) geometry, (3) biodegradability, (4) biomolecules delivery, (5) mechanical competence, which is generally seen as a problem. Herein, we developed silicon-wollastonite bioceramic based composite scaffolds with high strength via selective laser melting which can be easily tailored with shape and size to the diseased or injured area avoiding the binder addition and post-processing stages. As a result, the scaffold with a circular pore size of 400 um and porosity of approximately 35.2% exhibited a high compressive strength of 110 MPa (cortical bone defects). Moreover, finite element simulation results were in good agreement with the experimental results. Additionally, local delivery of vancomycin and bone morphogenetic proteins (BMPs) were also studied through the as-synthesized bioceramic scaffolds and promising results were observed. These findings demonstrate that as-synthesized composite scaffolds can pave the way for treating dental and maxillofacial defects too for large load-bearing repair applications.

10:50 AM

(BIO-112-2019) Microstructure-Electrical Properties Correlation of Pressureless Sintered Al_2O_3-$CaTiO_3$ Nanocomposite (Invited)

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Alumina (Al_2O_3) is a biologically inert ceramic that limits the bone growth in vitro and in vivo. But its good mechanical properties enables for load-bearing hard tissue replacement. In contrast, calcium titanate ($CaTiO_3$) is a good bioactive, osseointegration and osteoinductivity than HA. Our main objective is to determine the microstructure–electrical properties correlation of Al_2O_3-$CaTiO_3$ (ACT) composites using impendence analyser. A range of ACT composites was developed by pressureless sintering process. Phase identification and microstructural analysis were carried by XRD and SEM. AC conductivity and permittivity were carried out by using impendence analyser as the function of frequency and temperature from 100 KHz–1MHz and RT to 200ºC. As a result, 98% theoretical density was achieved for ACT composite sintering temperature at 1400ºC for 2 hours. XRD analysis was revealed the absence of $CaAl_2O_3$ phase. The activation energy was calculated from the Arrhenius plot indicatesthe linearity and a non-Debye type relaxation due to the conduction process are not thermally activated. Finally, it can be suggested that the developed nanocomposite could be used for the interfacing materials in bioelectronicsand biomaterial applications.

11:20 AM

(BIO-113-2019) Mineralization of Cell-Hydrogel Constructs: The Benefits of Ultrasound-derived Acoustic Radiation Force on Bone Repair (Invited)

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2. University of Connecticut, Materials Science and Engineering, USA
3. University of Connecticut, BIomedical Engineering, USA

Healing of large-scale bone defects remains an unsolved clinical challenge in the orthopaedic realm. Clinical strategies like autografts, allografts, and bone graft substitutes, and preclinical strategies like tissue engineering, and regenerative medicine all have viability as solutions to this challenge and many have been implemented with varying degrees of success. We have sought to combine both clinical and preclinical strategies into a solution for healing large-scale defects by combining cell delivery via a biocompatible, biodegradable hydrogel with low intensity pulsed ultrasound (LIPUS), a clinically proven method of reducing fracture healing time, into one approach that permits the implantation of cell-laden hydrogels into large-scale bone defects followed by intermittent transdermal application of LIPUS-derived acoustic radiation force (ARF) to the implanted cells. Our work has shown elevated levels of mineralization in hydrogels loaded with marrow-derived stem cells and exposed to ARF over the same cells with no ARF. We have also shown the ability to modulate the extent of mineralization by varying the ultrasound intensity and hydrogel composition. This has the potential of becoming a viable tool for healing large scale bone defects within the clinical orthopaedic realm.

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