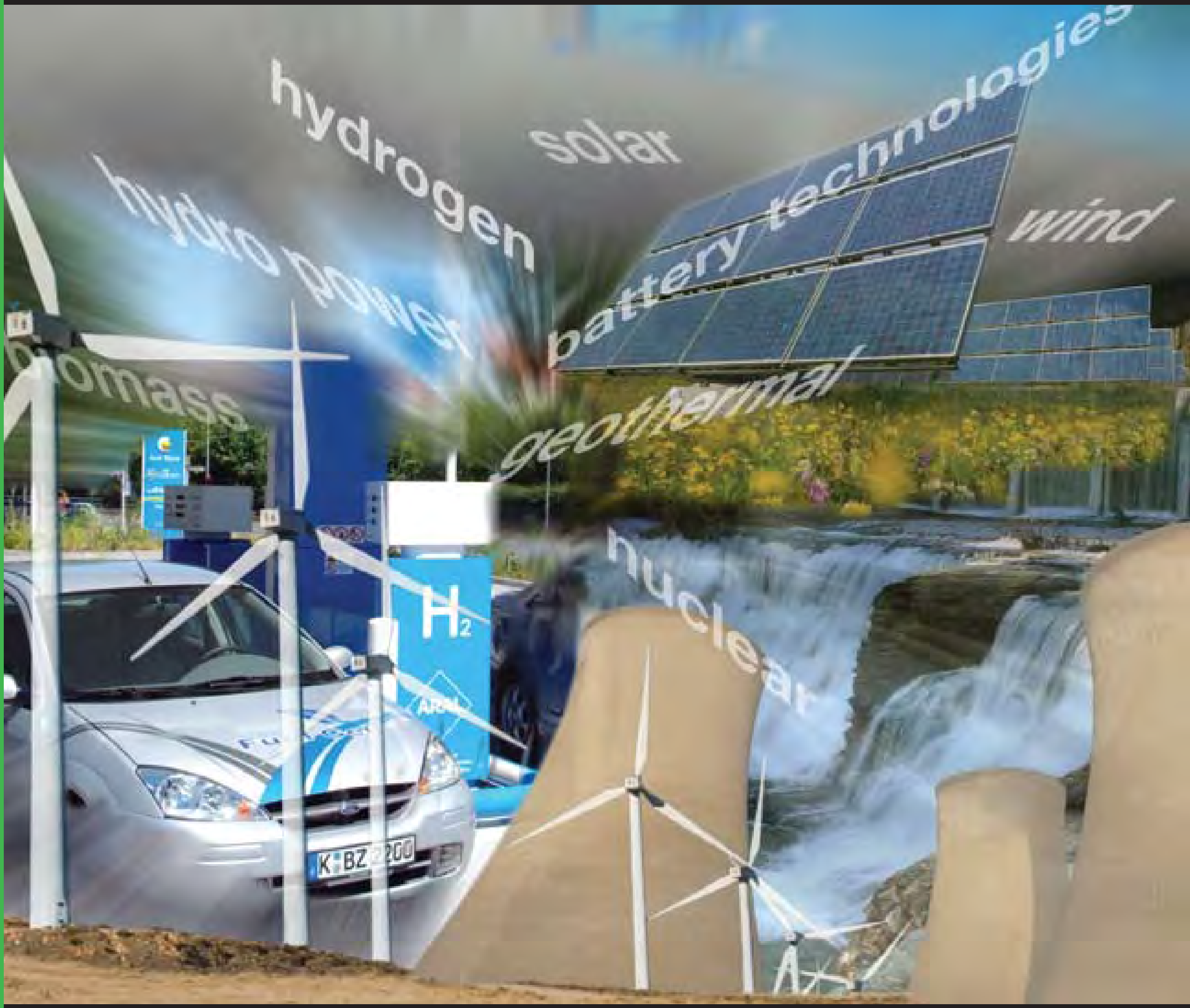
Meeting Guide



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www.ceramics.org

ASM International
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MRS Materials Research Society

MATERIALS CHALLENGES IN ALTERNATIVE & RENEWABLE ENERGY

February 21-24, 2010
Hilton Cocoa Beach Oceanfront | Cocoa Beach, Florida, USA

INSTITUTE OF METAL RESEARCH
CHINESE ACADEMY OF SCIENCES

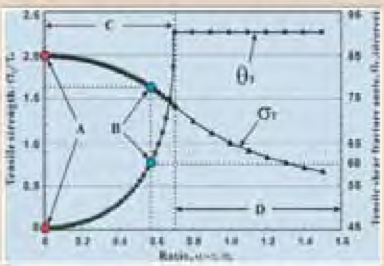
Website: http://www.imr.cas.cn

The Institute of Metal Research (IMR), Chinese Academy of Sciences (CAS) was founded in 1953, and the first term Director was Prof. Hsun Lee. The new IMR was formed in 1999 by merging with the former Institute of Corrosion and Protection of Metals (ICPM) of the Chinese Academy of Sciences which was established in 1982. The IMR is one of the most important R & D institution for materials science and engineering in China.

The IMR is mainly engaged in research and development of high performance metallic materials, new inorganic nonmetallic materials and advanced composite materials covering their structures, properties, performances, corrosion and protection, as well as the relationship among them. IMR pays equal attention to materials engineering such as synthesis, fabrication, processing and applications.

Nanostructured twin copper with ultrahigh strength and high electrical conductivity

Presently IMR has the first national laboratory in China, one state key laboratory, sixteen research divisions, two national engineering research centers and several spin-off high-tech enterprises. These include the Shenyang National Laboratory for Materials Science (SYNL, ten research divisions), the State Key Laboratory for Corrosion and Protection of Metals, the Shenyang Research and Development Center for Advanced Materials (seven research divisions), the Research Center for Environmental Corrosion of Materials, the National Engineering Research Center for Homogenized Alloys, the National Engineering Technology Center for Corrosion Control, and Shenyang Kejin New Materials Corporation, Ltd.



Schematic illustration of the ellipse criterion at different conditions

In recent years, IMR has made great achievements in the field of materials physics, non-equilibrium materials and nano-materials, machinable advanced ceramics, special materials for crucial environment, high temperature titanium alloys, superalloys, SiC foams, energy materials, computer simulations, materials processing and materials protection techniques. In 2005-2008, 1989 articles were published in international journals and 495 patents were obtained.

The IMR carries out extensive research works on energy materials including IN690, IN718, 1Cr13 and ceramic materials for nuclear power plants, superalloys and TiAl intermetallic compounds for turbine blades, new energy storage and hydrogen storage materials, as well as other materials and devices. Besides the materials research, attention also has been paid to the energy engineering including the material processing of huge casting and forging parts used in hydraulic turbine runners and vessels in nuclear power plants.

IMR develop various corrosion control methodologies and have been applying its techniques in industries. As a example, the Hangzhou Bay bridge with 36 km long used IMR’ s heavy corrosion protection coatings, cathodic protection tech., the corrosion sensors and in-situ monitoring techniques to insure 100 years lifetime.

The IMR currently has permanent staff of more than 800, including 8 CAS and CAE Members, 101 Professors, 93 Associate Professors and 76 Senior Engineers. In addition, there are more than 600 graduate students pursuing for Ph. D and Master degree, 30 postdoctoral fellows and 40 visiting scientists.

Hydraulic turbine runner in Three Gorge power station

IMR has close relationships with institutions, universities and academic associations from more than 30 countries and regions to carry out scientific exchanges and co-operations. There are 18 scientists holding positions in 49 international academic organizations or journals, such as editors and associate editors of Scripta Materialia, Carbon, J. of American Ceramic Society, etc.

IMR edits and publishes six key academic periodicals on materials science and engineering, including Acta Metallurgica Sinica (both in Chinese and English), Journal of Materials Science & Technology (in English), Chinese Journal of Materials Research, and Journal of Chinese Society for Corrosion and Protection.

Finally, the mission of IMR is to excel in materials research, develop advanced materials technology and foster exceptional talents, serving the nation, the society and mankind.

Welcome

Welcome to the Materials Challenges in Alternative & Renewable Energy Conference (Energy 2010). Designed to bring together leaders in materials science and energy, Energy 2010 aims to facilitate information sharing on the latest developments involving materials for alternative and renewable energy sources and systems.

We are happy that three of the premier materials organizations - The American Ceramic Society (ACerS), ASM International, and Society of Plastics Engineers (SPE) - representing the disciplines of ceramics, metals and polymers, have joined forces to co-sponsor this conference of global importance. In addition, we are pleased to have the endorsement of the Materials Research Society (MRS) and the Society for the Advancement of Material and Process Engineering (SAMPE).

The objective of Energy 2010 is to bring together leaders in materials science and energy to share information and the latest developments involving materials for alternative and renewable energy sources and systems. The conference includes nine "tutorial" presentations on leading energy alternatives that will be given by global leaders in the field. In addition, the conference includes technical sessions addressing state-of-the art materials challenges involved with Solar, Wind, Hydropower, Geothermal, Biomass, Nuclear, Hydrogen, and Batteries and Energy Storage.

This meeting was designed for scientists and engineers who are active in energy and materials science as well as those who are new to the field. The overall efficiency, effectiveness and practicality of potential future energy source and systems are directly related to many materials related factors. Some of these key features include materials costs, availability and improvements in chemical, mechanical, electrical and/or thermal properties of materials now being considered, as well as the ability to produce and fabricate materials in forms and shapes that work effectively in areas of energy generation, storage and distribution.

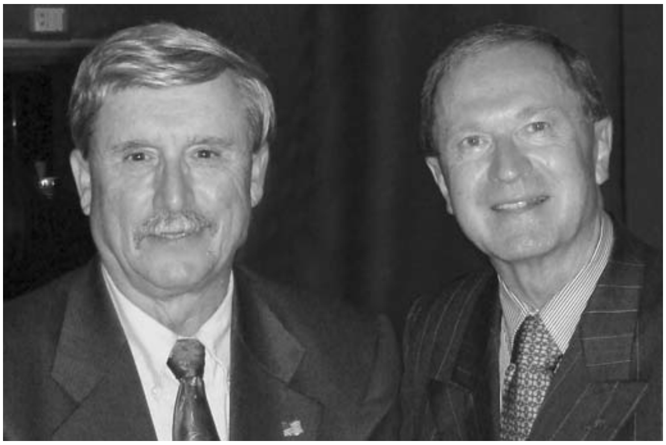
We are very excited that ACerS is committed to running this conference every two years. We believe the conference will grow in importance, size, and effectiveness for the materials community.

Best regards,

George and Jack

George Wicks
Savannah River National Laoboratory

Jack Simon
Technology Access



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MEETING REGULATIONS

The American Ceramic Society is a nonprofit scientific organization that facilitates the exchange of knowledge meetings and publication of papers for future reference. The Society owns and retains full right to control its publications and its meetings. The Society has an obligation to protect its members and meetings from intrusion by others who may wish to use the meetings for their own private promotion purpose. Literature found not to be in agreement with the Society's goals, in competition with Society services or of an offensive nature will not be displayed anywhere in the vicinity of the meeting. Promotional literature of any kind may not be displayed without the Society's permission and unless the Society provides tables for this purpose. Literature not conforming to this policy or displayed in other than designated areas will be disposed. The Society will not permit unauthorized scheduling of activities during its meeting by any person or group when those activities are conducted at its meeting place in interference with its programs and scheduled activities. The Society does not object to appropriate activities by others during its meetings if it is consulted with regard to time, place, and suitability. Any person or group wishing to conduct any activity at the time and location of the Society meeting must obtain permission from the Executive Director, giving full details regarding desired time, place and nature of activity.

Registration Requirements: Attendance at any meeting of the Society shall be limited to duly registered persons.

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Final determination of the suitability of any information, procedure or products for use contemplated by any user, and the manner of that use, is the sole responsibility of the user. Expert advice should be obtained at all times when implementation is being considered, particularly where hazardous materials or processes are encountered.

Organizing Committee

Conference Co-Chairs
Dr. George Wicks, Savannah River National Laboratory, Aiken, SC
Dr. Jack Simon, Technology Access, Aiken, SC

Advisory & Technical Planning Committee:
Dr. Jack Simon, Technology Access and Alpha Sigma Mu Honorary Society
Dr. George Wicks, Savannah River National Lab
Dr. Thad Adams, Savannah River National Lab
Dr. Joel Ager, Lawrence Berkeley National Lab
Dr. Ming Au, Savannah River National Lab
Dr. Amir Farajian, Wright State Univ.
Ms. Rita Forman-House, ASM International
Dr. Brenda Garcia-Diaz, Savannah River National Lab
Dr. Frank Goldner, U.S. Dept. of Energy
Prof. Hong Huang, Wright State Univ.
Dr. M. Ashraf Imam, Naval Research Lab
Dr. Natraj Iyer, Savannah River National Lab
Prof. Puru Jena, Virginia Commonwealth Univ.
Dr. Enamul Haque, Bostik, Inc.
Dr. Abhi Karkamkar, Pacific Northwest National Lab
Dr. Gene Kim, Cookson Electronics
Ms. Lesley Kyle, Society for Plastics Engineers (SPE)
Dr. Edgar Lara-Curzio, Oak Ridge National Lab
Mr. Richard Marczewski, Savannah River National Lab
Dr. Rana Mohtadi, Toyota Technical Center, NA
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Dr. Bhakta Rath, Naval Research Lab
Dr. Robert Sindelar, Savannah River National Lab
Prof. Rick Sisson, Worcester Polytechnic Institute
Ms. Hidda Thorsteinsson, U.S. Dept. of Energy
Ms. Agatha Wein, U.S. Dept. of Energy
Mr. Jose Zayas, Sandia National Labs
Dr. Kristine Zeigler, Savannah River National Lab
Dr. Ragaiy Zidan, Savannah River National Lab
Mr. Mark Mecklenborg, The American Ceramic Society
Mr. Greg Geiger, The American Ceramic Society

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Schedule At A Glance

Sunday, February 21, 2010

Conference Registration	3 PM – 7 PM	Grand Ballroom Foyer
Welcome Reception	5 PM – 7 PM	Pool Deck

Monday, February 22, 2010

Conference Registration	7 AM – 7:30 PM	Grand Ballroom Foyer
Welcome and Tutorial Lectures	8:15 AM – 12:15 PM	Sea Oats & Sawgrass
Lunch	12:15 PM – 2 PM	Horizons
Tutorial Lectures	2 PM – 5:30 PM	Sea Oats & Sawgrass
Pre-Conference Dinner Reception	7 PM – 7:30 PM	Grand Ballroom Foyer
Dinner	7:30 PM – 9:30 PM	Grand Ballroom

Tuesday, February 23, 2010

Conference Registration	7 AM – 5:30 PM	Grand Ballroom Foyer
Concurrent Technical Sessions	8 AM – 12 PM	
Lunch On Own	12 PM – 1:40 PM	
Concurrent Technical Sessions	1:40 PM – 5 PM	
Poster Session Set-Up	3 PM – 5:30 PM	Horizons
Dinner On Own	5:30 PM – 7 PM	
Poster Session and Reception	7 PM – 9 PM	Horizons

Wednesday, February 24, 2010

Conference Registration	7:30 AM – 4:30 PM	Grand Ballroom Foyer
Concurrent Technical Sessions	8 AM – 12 PM	
Lunch On Own	12 PM – 1:40 PM	
Concurrent Technical Sessions	1:40 PM – 5 PM	

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National Renewable Energy Laboratory

Technical Sessions by Symposium

Session Title	Day	Time	Location
Tutorial Session	Monday, February 22	8:15 - 5:30 PM	SeaOats/Sawgrass/ Dunes 1&2

Batteries and Energy Storage Materials

Energy Storage and Conversion I	Tuesday, February 23	8 AM - 12 Noon	Sawgrass
Energy Storage and Conversion II	Wednesday, February 24	8 AM - 12:20 PM	Sawgrass
Energy Storage and Conversion III	Wednesday, February 24	1:40 - 4:40 PM	Sawgrass

Biomass

Materials Compatibilty with Biofuels	Wednesday, February 24	8 AM - 12 Noon	Dunes 1&2

Geothermal/HydroPower

Materials Challenges in Hydro and Geothermal Energy	Wednesday, February 24	1:40 - 4:40 PM	Sea Oats

Hydrogen

High Capacity Materials for Hydrogen Storage	Tuesday, February 23	8 AM - 12 Noon	Seashore Ballroom
Processing and Applications for Hydrogen Storage	Tuesday, February 23	1:40 - 5:00 PM	Seashore Ballroom
Nanostructures and Catalytic Materials for Hydrogen Storage	Wednesday, February 24	8 AM - 12 Noon	Seashore Ballroom
Characterization and Analysis of Hydrogen Storage Materials	Wednesday, February 24	1:40 - 5:00 PM	Seashore Ballroom

Nuclear

Nuclear Fuels	Tuesday, February 23	8 AM - 12 Noon	Dunes 1&2
Waste Forms	Tuesday, February 23	1:40 - 5:00 PM	Dunes 1&2
Modeling and Simulation	Wednesday, February 24	1:40 - 4:20 PM	Dunes 1&2

Solar

Coating and Silicon Based PVs	Tuesday, February 23	8 AM - 12 Noon	Sea Oats
Dye Sensitized Solar Cells and Copper Indium Gallium Selenide based Photovoltaics	Tuesday, February 23	1:40 - 5:00 PM	Sea Oats

Wind

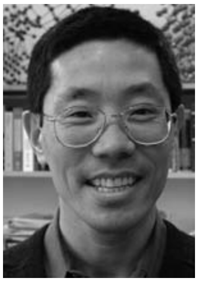
Materials Trends and Opportunities for Wind Energy Applications	Wednesday, February 24	8 AM - 12 Noon	Sea Oats

Tutorial Speakers

Batteries & Energy Storage

Yet-Ming Chiang, Massachusetts Institute of Technology

Title: Advances in Battery Technology



Yet-Ming Chiang is Kyocera Professor of Ceramics in the Department of Materials Science and Engineering at MIT, where he has been a faculty member since 1984. He is a member of the National Academy of Engineering. His research and teaching focuses on advanced materials and their role in technologies for energy storage and generation, medical devices, "smart" structures, and micro/nano electronics. Basic research from his laboratory enabled new battery technology that received in 2006 an R&D 100 Award and the R&D 100 Editor's Choice Award. He is the founding scientist of A123Systems, a pioneer in high power, long life rechargeable battery technology used in cordless power tools, hybrid and plug-in hybrid electric vehicles, grid stabilization, and other developing energy storage applications.

Hydrogen

Ned Stetson, U.S. Department of Energy (DOE)

Title: Achievements and Perspectives of the US National Program on Hydrogen Storage

Dr. Stetson is a Technology Development Manager for the U.S. Department of Energy's Hydrogen Program with over 18 years of experience in hydrogen storage materials and technology development. Stetson manages hydrogen storage projects, including the Metal Hydride Center of Excellence and the H-Prize. Prior to joining, he researched complex hydrides at the Univ. of Geneva. Stetson also spent over 10 years at ECD-Ovonics, where he was involved with the development of novel hydrogen storage materials and hydride-based hydrogen storage systems. He has also been active with the Compressed Gas Association, Society of Automotive Engineers, International Code Council and the International Standards Organization.

Solar

Ryne Raffaelle, National Renewable Energy Lab (NREL)

Title: Photovoltaics: Past, Present and Future

Dr. Raffaelle is the Director of the National Center for Photovoltaics at NREL. Previously, Raffaelle was the Academic Director for the Golisano Institute for Sustainability and Director of the NanoPower Research Laboratory at Rochester Institute of Technology (RIT) in New York. While directing the two institutions at RIT, he also served as a professor of physics, microsystems engineering and sustainability and was responsible for $20 million in research grants in photovoltaics, thin-film processing, and nanomaterials research. He co-founded two photovoltaic and power system start-up companies, authored or co-authored over 150 refereed publications, and has served on the organizing committee for the past four IEEE Photovoltaics Specialists Conferences and the last World Conference.

Wind

Jose R. Zayas, Sandia National Labs (SNL)

Title: Wind: Background, Technology Opportunities, and Material Challenges

Mr. Zayas is the program manager of the Wind and Water Power Technologies Department at Sandia National Laboratories. He joined Sandia in 1996, and has over 13 years of wind energy experience. During his career he's performed research in a variety of areas which include active aerodynamic flow control, sensors, dynamic modeling, data acquisition systems, and component testing. Jose holds a bachelors degree in Mechanical Engineering from the University of New Mexico, and a Masters degree in Mechanical and Aeronautical Engineering from the University of California.

Nuclear

Steve Zinkle, Oak Ridge National Lab (ORNL)

Title: Materials Challenges in Nuclear Energy

Dr. Zinkle is a Corporate Fellow and director of the Materials Science and Technology Division at Oak Ridge National Laboratory. He has written over 230 peer-reviewed publications, is a fellow of the American Ceramic Society, ASM International, and the American Nuclear Society, and received the U.S. Department of Energy 2006 E.O. Lawrence Award.

General

Mark Verbrugge, General Motors Research & Development Center

Title: Material Needs in Alternative & Renewable Energy for the Automotive Industry

Dr. Verbrugge is the Director of Chemical Sciences and Materials System Laboratory, General Motors Research & Development. He began his GM career in 1986 with the GM Research Labs after receiving his doctorate in Chemical Engineering from University of California-Berkeley. Verbrugge has published and patented in areas of electroanalytical methods, polymer electrolytes, advanced batteries and supercapacitors, fuel cells, high-temperature air-to-fuel-ratio sensors, surface coatings, compound semiconductors, and automotive applications of structural materials. Verbrugge is a Board Member of the U.S. Automotive Materials Partnership LLC and the U.S. Advanced Battery Consortium LLC, and an adjunct professor for the Department of Physics, University of Windsor.

General

Kevin Billings, Lockheed Martin

Title: Striking A Balance To Allow The Defense Industry To Fully Participate In Meeting Alternative And Renewable Energy Goals

Mr. Billings is Director of Federal Energy Management Programs at Lockheed Martin. Most recently, he was Acting Assistant Secretary of the Air Force for Installations, Environment and Logistics. As the Acting Assistant Secretary, he led the $38 billion three division department responsible for Air Force facility and logistical issues world-wide.

General

Gary Wright, Air Force Research Lab

Title: Air Force Energy Strategy

Mr. Wright is a Research Engineer at the Air Force Research Laboratory (AFRL). Mr. Wright served 22 years on active duty in the Air Force and retired in 2008. At AFRL, one of his research interests is defining strategies to implement renewable energy technologies with a net-zero environmental impact.

General

Sandra DeVincent Wolf, MRS

Title: Advanced Materials for Our Energy Future: Study Results

Ms. DeVincent Wolf currently serves MRS as Director of Membership Development and is responsible for developing strategic approaches to membership programs, coordinating advocacy and outreach initiatives, and creating key services for the materials community. She has a background in Materials Science and Engineering from the Massachusetts Institute of Technology and Case Western Reserve University, as well as 15 years of prior work experience in many sectors including government labs, small start-up companies and large corporations.

Oral Presenters

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Presenting Author List

Oral Presenters

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Name	Date	Time	Room	Page Number
Saxena, S.	23-Feb	3:40PM	Seashore Ballroom	14
Schubert, H.	23-Feb	11:00AM	Sawgrass	12
Schubert, P.J.	23-Feb	11:40AM	Sea Oats	11
Selvamanickam, V.	23-Feb	4:00PM	Sea Oats	13
Shaw, L.	24-Feb	9:20AM	Seashore Ballroom	15
Sindelar, R.L.	23-Feb	2:20PM	Dunes 1&2	14
Srinivasan, R.	24-Feb	4:20PM	Sawgrass	18
Stan, M.	24-Feb	2:00PM	Dunes 1&2	18
Stanek, C.	24-Feb	3:40PM	Dunes 1&2	18
Stavila, V.	23-Feb	8:40AM	Seashore Ballroom	12
Stetson, N.T.	22-Feb	9:15AM	SeaOats/Sawgrass/Dunes 1&2	11
Stowe, A.C.	24-Feb	4:40PM	Seashore Ballroom	17
Summers, W.A.	23-Feb	1:40PM	Seashore Ballroom	13
Sundararajan, G.	23-Feb	11:40AM	Dunes 1&2	13

T

Name	Date	Time	Room	Page Number
Tiwari, G.P.	23-Feb	2:20PM	Seashore Ballroom	14
Toloczko, M.	23-Feb	9:20AM	Dunes 1&2	13
Tupper, M.	23-Feb	11:20AM	Sea Oats	11
Tupper, M.	23-Feb	4:40PM	Seashore Ballroom	14
Tupper, M.	24-Feb	2:20PM	Sea Oats	18
Tupper, M.	24-Feb	4:20PM	Sea Oats	18
Tupper, M.	24-Feb	8:40AM	Sea Oats	17

V

Name	Date	Time	Room	Page Number
van Swol, F.	24-Feb	9:00AM	Seashore Ballroom	15
Verbrugge, M.	22-Feb	2:15PM	SeaOats/Sawgrass/Dunes 1&2	11
Voit, S.	23-Feb	8:40AM	Dunes 1&2	13

W

Name	Date	Time	Room	Page Number
Walker, G.	23-Feb	11:20AM	Seashore Ballroom	12
Wan, X.	23-Feb	9:20AM	Seashore Ballroom	12
Wang, P.	24-Feb	2:40PM	Sea Oats	18
Wang, Y.	23-Feb	4:40PM	Dunes 1&2	14
Wright, G.	22-Feb	4:00PM	SeaOats/Sawgrass/Dunes 1&2	11

X

Name	Date	Time	Room	Page Number
Xiong, Z.	23-Feb	9:00AM	Seashore Ballroom	12

Z

Name	Date	Time	Room	Page Number
Zare, M.	23-Feb	11:00AM	Sea Oats	11
Zayas, J.	22-Feb	11:00AM	SeaOats/Sawgrass/Dunes 1&2	11
Zidan, R.	23-Feb	10:20AM	Seashore Ballroom	12
Zidan, R.	24-Feb	10:40AM	Seashore Ballroom	15
Zinkle, S.J.	22-Feb	11:45AM	SeaOats/Sawgrass/Dunes 1&2	11
Zukalova, M.	23-Feb	9:40AM	Sawgrass	12

Poster Presenters

Name	Date	Time	Room	Page Number
Balandeh, M.	23-Feb	7:00PM	Horizons	14
Chen, W.M.	23-Feb	7:00PM	Horizons	15
Dominguez, O.	23-Feb	7:00PM	Horizons	14
Dunwoody, J.T.	23-Feb	7:00PM	Horizons	15
Halloran, J.	23-Feb	7:00PM	Horizons	15
Hong, Y.	23-Feb	7:00PM	Horizons	14
Karkamkar, A.	23-Feb	7:00PM	Horizons	15
Kastner, J.	23-Feb	7:00PM	Horizons	15
Kim, S.	23-Feb	7:00PM	Horizons	14
Lee, J.A.	23-Feb	7:00PM	Horizons	15
Levchenko, A.	23-Feb	7:00PM	Horizons	14
Ma, Z.	23-Feb	7:00PM	Horizons	15
Myung, J.	23-Feb	7:00PM	Horizons	15
Narase Gowda, S.	23-Feb	7:00PM	Horizons	15
Ortega, L.H.	23-Feb	7:00PM	Horizons	14
Shaban, H.	23-Feb	7:00PM	Horizons	15
Thanganathan, U.	23-Feb	7:00PM	Horizons	15
Ukpai, W.D.	23-Feb	7:00PM	Horizons	15
Usov, I.	23-Feb	7:00PM	Horizons	14
Varma, A.	23-Feb	7:00PM	Horizons	15
Volobujeva, O.	23-Feb	7:00PM	Horizons	15
Wang, J.	23-Feb	7:00PM	Horizons	15
Willson, S.P.	23-Feb	7:00PM	Horizons	14
Yen, C.	23-Feb	7:00PM	Horizons	15

Monday, February 22, 2010

Tutorial Session

Room: SeaOats/Sawgrass/Dunes 1&2

8:15 AM

Opening Remarks
George Wicks, SRNL

Jack Simon, Technology Access

8:30 AM

(ENERGY-001-2010) Advances in Battery Technology (Invited)
Y. Chiang*, Massachusetts Institute of Technology, United States

9:15 AM

(ENERGY-002-2010) Achievements and Perspectives of the US National Program on Hydrogen Storage (Invited)
N. T. Stetson*, C. Read, S. Dillich, G. Ordaz, M. Gardiner, R. Bowman, U.S. Department of Energy, United States

10:00 AM

Break

10:15 AM

(ENERGY-003-2010) Photovoltaics: Past, Present, and Future (Invited)
R. P. Raffaelle*, National Renewable Energy Lab, United States

11:00 AM

(ENERGY-004-2010) Wind Energy: Background, Technology Opportunities, and Material Challenges (Invited)
J. Zayas*, Sandia National Laboratories, United States

11:45 AM

(ENERGY-005-2010) Materials Challenges in Nuclear Energy (Invited)
S. J. Zinkle*, Oak Ridge National Laboratory, United States

12:30 PM

Lunch

2:15 PM

(ENERGY-006-2010) Material Needs in Alternative and Renewable Energy for the Automotive Industry (Invited)
M. Verbrugge*, GM R&D, United States

3:00 PM

(ENERGY-007-2010) Striking a Balance to Allow the Defense Industry to Fully Participate in Meeting Alternative and Renewable Energy Goals (Invited)
K. Billings*, Lockheed Martin, United States

3:45 PM

Break

4:00 PM

(ENERGY-008-2010) Air Force Energy Strategy (Invited)
G. Wright*, AFRL, United States

4:45 PM

(ENERGY-009-2010) Advanced Materials for Our Energy Future: Study Results (Invited)
S. DeVincent Wolf*, Materials Research Society, United States; D. Dimos, Sandia National Laboratories, United States

Tuesday, February 23, 2010

Solar

Coating and Silicon Based PVs

Room: Sea Oats

Session Chair: Abhi Karkamkar, Pacific Northwest National Lab

8:00 AM

(ENERGY-010-2010) Silicone Materials for Photovoltaic Module Assembly
A. Norris*, M. Tomalia, B. Ketola, Dow Corning Corporation, United States

8:20 AM

(ENERGY-011-2010) Biomimetic Nanostructured Anti-Reflection Coatings for Highly Efficient Solar Cells
M. Kane*, Savannah River National Laboratory, United States; P. Jiang, University of Florida, United States

8:40 AM

(ENERGY-012-2010) Novel Resilient Flux Coated ReadyRibbonTM Solder Ribbon for Polysilicon Photovoltaic Cell Module Assembly
G. Kim*, M. Marczi, G. Cunning, O. Khaselev, Cookson Electronics Assembly Materials Group, United States

9:00 AM

(ENERGY-013-2010) Vapor-liquid-solid grown silicon nanowire solar cells
J. Greil*, A. Lugstein, E. Bertagnolli, Vienna University of Technology, Austria

9:20 AM

(ENERGY-014-2010) Synthesis of Solar-grade Silicon from Amorphous Silica (Rice Husk Ash)
K. K. Larbi*, M. Barati, A. McLean, R. Roy, University of Toronto, Canada

9:40 AM

(ENERGY-015-2010) Rice Hulls to Solar Grade Silicon
M. Mede*, Thermal Technology LLC, United States; P. Italiano, Costech International s.P.a., Italy; S. Cooke, Solution Research, United States

10:00 AM

Break

10:20 AM

(ENERGY-016-2010) Metallurgical Refining of Silicon for Solar Applications by Slagging of Impurity Elements
M. Johnston*, M. Barati, University of Toronto, Canada

10:40 AM

(ENERGY-017-2010) A Novel Purification Method for Production of Solar Grade Silicon
S. Esfahani*, M. Barati, Z. Yin, University of Toronto, Canada

11:00 AM

(ENERGY-018-2010) Thermal heat storage in inorganic molten salt slurries for solar central electricity
M. Zare*, R. Abbaschian, University of California, Riverside, United States

11:20 AM

(ENERGY-019-2010) Advanced Composite Materials Enable Effective Energy Capture from Thin Film and High Efficiency Solar Cells
M. Tupper*, P. Keller, R. Taylor, R. Barrett, D. Turse, W. Francis, CTD, United States

11:40 AM

(ENERGY-020-2010) Materials Selection and Processing for Lunar-based Space Solar Power
P. J. Schubert*, Packer Engineering, Inc., United States

Hydrogen

High Capacity Materials for Hydrogen Storage

Room: Seashore Ballroom

Session Chairs: Ewa Ronnebro, Pacific Northwest National Laboratory; Ragaiy Zidan, Savannah River National Laboratory

8:00 AM

(ENERGY-021-2010) Development of Processes for the Reversible Dehydrogenation of High Hydrogen Capacity Complex Hydrides (Invited)
G. Severa, University of Hawaii at Manoa, United States; E. Ronnebro, Sandia National Laboratories, United States; X. Liu, G. McGrady, H. Langmi, University of New Brunswick, Canada; C. M. Jensen*, University of Hawaii at Manoa, United States

8:20 AM

(ENERGY-022-2010) Development of hybrid tank system and investigation of hydrogen absorbing alloys
E. Akiba*, K. Asano, AIST, Japan; T. Fuura, S. Tsunokake, Japan Metals and Chemicals, Japan; Y. Sakaguchi, SAMTECH, Japan; M. Monde, Saga University, Japan

8:40 AM

(ENERGY-023-2010) Factors Affecting Hydrogen Release from Metal Borohydrides
V. Stavila*, Sandia National Laboratories, United States; E. H. Majzoub, University of Missouri, United States; S. Hwang, California Institute of Technology, United States; R. J. Newhouse, University of California Santa Cruz, United States; M. Ulutagay-Kartin, W. Luo, J. G. Cordaro, Sandia National Laboratories, United States; T. J. Udovic, National Institute of Standards and Technology, United States

9:00 AM

(ENERGY-024-2010) Synthesis of alkali amidoborane for hydrogen storage
Z. Xiong*, G. Wu, J. Guo, H. Chu, C. Wu, Dalian Institute of Chemical Physics, China; Y. Chua, National University of Singapore, Singapore; P. Chen, Dalian Institute of Chemical Physics, China

9:20 AM

(ENERGY-025-2010) Enhancing the Hydriding and Dehydriding Kinetics of $LiBH_4$+MgH_2 Systems via the Addition of Transition Metals
X. Wan*, K. Crosby, Y. Zhong, L. L. Shaw, University of Connecticut, United States

9:40 AM

(ENERGY-026-2010) Adduct-stabilized aluminum borohydride as advanced hydrogen storage materials
D. A. Knight*, R. Zidan, C. Fewox, T. Motyka, Savannah River National Laboratory, United States; R. Mohtadi, P. Sivasubramanian, Toyota Research Institute of North America, United States

10:00 AM

Break

10:20 AM

(ENERGY-027-2010) Forming and Regenerating Alane using Electrochemical Cycle (Invited)
R. Zidan*, Savannah River National Laboratory, United States

10:40 AM

(ENERGY-028-2010) Tuning complex metal hydrides properties for onboard hydrogen storage application (Invited)
R. Mohtadi*, P. Sivasubramanian, Toyota Research Institute of North America, United States; J. Gray, R. Zidan, Savannah River National Laboratory, United States

11:00 AM

(ENERGY-029-2010) Solid State Chemical Hydrogen Storage in NHxBHx Materials (Invited)
A. Karkamkar, T. Autrey*, Pacific Northwest National Laboratory, United States

11:20 AM

(ENERGY-030-2010) Multicomponent hydrogen storage materials based on LiBH4 (Invited)
G. Walker*, University of Nottingham, United Kingdom

11:40 AM

(ENERGY-031-2010) Decomposition behaviour of metal borohydride compounds (Invited)
D. Book*, D. Reed, University of Birmingham, United Kingdom

Battery Technology

Energy Storage and Conversion I

Room: Sawgrass

Session Chair: Thad Adams, Savannah River National Lab

8:00 AM

(ENERGY-032-2010) Free Standing Nanostructured Anodes for Li-Ion Batteries (Invited)
M. Au*, T. Adams, Savannah River National Laboratory, United States; Y. Zhao, University of Georgia, United States

8:40 AM

(ENERGY-033-2010) Modeling nanoparticle synthesis by gas condensation in a nanocluster source for applications in photovoltaic and hydrogen fuel cells
E. Pauliac-Vaujour*, E. Quesnel, V. Muffato, CEA Grenoble, France

9:00 AM

(ENERGY-034-2010) Nano-aggregate synthesis by gas condensation in a magnetron source for efficient energy conversion devices
E. Pauliac-Vaujour*, E. Quesnel, V. Muffato, R. Najjar, N. Baclet, R. Bouchmila, P. Fugier, CEA Grenoble, France

9:20 AM

(ENERGY-035-2010) Multi-walled Carbon Nanotubes Functionalized by Carboxylic Groups: Activation of TiO2 (Anatase) and Phosphate Olivines (LiMnPO4, LiFePO4) for Electrochemical Li-storage
L. Kavan*, J HEYROVSKY INSTITUTE, Czech Republic

9:40 AM

(ENERGY-036-2010) Nanofibrous TiO2: A new material with extraordinary properties
M. Zukalova*, L. Kavan, J. Prochazka, JHIPCH, Czech Republic

10:00 AM

Break

10:20 AM

(ENERGY-037-2010) Ferrocene based carbon–Iron/lithium fluoride nanocomposite as stable electrode material in lithium batteries (Invited)
R. Prakash*, M. Fichtner, Karlsruhe Institute of Technology, Germany

11:00 AM

(ENERGY-038-2010) New Channel Structure Materials for Cathodes of Li Batteries: Processing and Structural Investigations
C. Kallfass, Max Planck Gesellschaft, Germany; S. Hermann, Technische Universität Berlin, Germany, Technische Universität Berlin, GermanyMax Planck Gesellschaft, Germany; H. Schubert*, Technische Universität Berlin, Germany

11:20 AM

(ENERGY-039-2010) Graphite coated with SiCN ceramic: can one explain the enhanced electrochemical properties of this anode material by understanding the lithium diffusion mechanism?
A. P. Nowak*, M. Graczyk-Zajac, C. Fasel, R. Riedel, Darmstadt University of Technology, Germany

11:40 AM

(ENERGY-040-2010) TiO2 Brookite as anode for lithium ion batteries
D. Dambournet*, I. Belharouak, K. Amine, Argonne National Laboratory, United States

Nuclear

Nuclear Fuels

Room: Dunes 1&2

Session Chairs: Robert Sindelar, Savannah River National Laboratory; Kenneth McClellan, Los Alamos National Lab

8:00 AM

(ENERGY-041-2010) Overview of Materials Challenges for Nuclear Fuels (Invited)
K. J. McClellan*, Los Alamos National Lab, United States

8:20 AM

(ENERGY-042-2010) Advanced Carbide and Nitride Nuclear Fuels (Invited)
J. Carmack*, S. L. Hayes, Idaho National Laboratory, United States

8:40 AM

(ENERGY-043-2010) Material Challenges for Particle Nuclear Fuel Technology
S. Voit*, G. DelCul, R. Hunt, Oak Ridge National Laboratory, United States

9:00 AM

(ENERGY-044-2010) Metal Fuel Development within the Fuel Cycle Research and Development Program (Invited)
J. Kennedy*, T. O'Holleran, J. I. Cole, D. E. Janney, R. Fielding, R. Mariani, C. Papesch, M. K. Fig, Idaho National Laboratory, United States

9:20 AM

(ENERGY-045-2010) Materials Issues in Cladding and Duct Reactor Materials
S. Maloy, LANL, United States; M. Toloczko*, PNNL, United States; J. Cole, INL, United States; T. Byun, ORNL, United States

9:40 AM

(ENERGY-046-2010) Chemical and Phase Behavior of Oxide Fuels for LWR and Fast Nuclear Reactors (Invited)
T. M. Besmann*, S. L. Voit, Oak Ridge National Laboratory, United States

10:00 AM

Break

10:20 AM

(ENERGY-047-2010) How Modeling and Simulation Helps Address Nuclear Fuels Challenges (Invited)
R. W. Grimes*, D. Parfitt, C. Bishop, Imperial College London, United Kingdom

10:40 AM

(ENERGY-048-2010) Microstructure Property Relations in Uranium Oxide
E. Luther*, D. Byler, K. McClellan, P. Papin, H. Volz, K. Lao, Los Alamos National Laboratory, United States

11:00 AM

(ENERGY-049-2010) Development of Capabilities for Thermal Analysis of Multilayer Materials for Advanced Nuclear Systems
A. T. Nelson*, Los Alamos National Laboratory, United States

11:20 AM

(ENERGY-050-2010) Effect of oxygen stoichiometry on the properties of uranium oxide fuels
D. D. Byler*, K. J. McClellan, E. P. Luther, P. A. Papin, H. M. Volz, Los Alamos National Laboratory, United States; J. B. Henderson, Netzsch Instruments North America, United States

11:40 AM

(ENERGY-051-2010) The Role of Titanium in Oxide Dispersion Strengthened Alloys for First Wall Structural Materials
G. Sundararajan*, R. Vijay, A. Venugopal Reddy, ARCI, India

Solar

Dye Sensitized Solar Cells and Copper Indium Gallium Selenide based Photovoltaics

Room: Sea Oats

Session Chair: Laura Marshall, ASM International

1:40 PM

(ENERGY-052-2010) Electrical Transport Properties of Lithographically Fabricated Single Titania Nanotube Devices
M. AbdElmoula*, L. Menon, Northeastern University, United States

2:00 PM

(ENERGY-053-2010) Composite of Nanoanatase Templated Structure and TiO2 Electrospun Nanofibers Improves Parameters of the DSC Anode
J. Prochazka*, L. Kavan, M. Zukalova, JHI, Czech Republic; M. Graetzel, EPFL, Switzerland

2:20 PM

(ENERGY-054-2010) Hybrid organic flexible solar collectors for smart building construction
J. Iroh*, B. Buschle, J. Logun, E. Obonyo, University of Cincinnati, United States

2:40 PM

(ENERGY-055-2010) Electrochemical Deposition of CoSb3 Thin Films on Nanostructured Substrate
D. V. Quach*, UC Davis, United States; R. Vidu, AMEROM LLC, United States; J. R. Groza, P. Stroeve, UC Davis, United States

3:00 PM

(ENERGY-056-2010) Suitability of Pyrolytic Boron Nitride, Hot Pressed Boron Nitride, and Pyrolytic Graphite for CIGS Processes
J. Mariner*, W. Fan, X. Liu, C. Raman, J. Leist, Momentive Performance Materials, United States

3:20 PM

Break

3:40 PM

(ENERGY-057-2010) Effect of Elemental Composition on Diffusion of Sulfur into $CuIn_xGa_{1-x}Se_2$ Thin Films
S. A. Pethe*, E. Takahashi, N. G. Dhere, Florida Solar Energy Center, University of Central Florida, United States

4:00 PM

(ENERGY-058-2010) III-V photovoltaics on flexible metal substrates using biaxially-textured Germanium films
V. Selvamanickam*, A. Freundlich, A. Sundaram, S. Lee, University of Houston, United States; S. Sambandam, A. Rar, X. Xiong, SuperPower, United States

4:20 PM

(ENERGY-059-2010) 200 MeV Ag+ ion beam induced modifications in AgInSe2 films deposited by hot wall vacuum evaporation method
D. Pathak*, R. K. Bedi, Guru Nanak Dev University, India; D. Kaur, Indian Institute of Technology, India; R. Kumar, Inter University Accelerator Centre, India

4:40 PM

(ENERGY-060-2010) Chemical Solution Deposition of IR-Active Thin Films: Epitaxial Growth and Carrier Multiplication
Y. Golan*, Ben Gurion University, Israel

Hydrogen

Processing and Applications for Hydrogen Storage

Room: Seashore Ballroom

Session Chairs: Theodore Motyka, Savannah River National Laboratory; Richard Sisson, Worcester Polytechnic Institute

1:40 PM

(ENERGY-061-2010) Large-scale Hydrogen Production by Nuclear Thermochemical Water-splitting (Invited)
W. A. Summers*, Savannah River National Laboratory, United States

2:00 PM

(ENERGY-062-2010) Hydrogen Storage in Glass Capillary Arrays
D. Eliezer*, C.En Ltd., Switzerland

2:20 PM

(ENERGY-063-2010) Stress Quenching of Hydrogen in AISI 403 Steel
G. P. Tiwari*, V. D. Alur, Bhabha Atomic Research Centre, India

2:40 PM

(ENERGY-064-2010) Production of hydrogen and carbon monoxide from water and carbon dioxide through metal oxide thermochemical cycles
E. N. Coker*, M. Rodriguez, A. Ambrosini, T. Garino, J. E. Miller, Sandia National Laboratories, United States

3:00 PM

(ENERGY-065-2010) Concentric Electrode-type On-planar Single-chamber Solid Oxide Fuel Cells
D. Lee*, Yonsei University, Korea, Republic of; H. Kim, Yonsei University, Korea, Republic of; J. Kim, KIST, Korea, Republic of; J. Moon, Yonsei University, Korea, Republic of

3:20 PM

Break

3:40 PM

(ENERGY-066-2010) A zero carbon emission method to produce hydrogen and hydrides (Invited)
S. Saxena*, S. Kumar, V. Drozd, FIU, United States

4:00 PM

(ENERGY-067-2010) Hydrogen storage materials properties for prototype system concepts (Invited)
E. Ronnebro*, Pacific Northwest National Laboratory, United States

4:20 PM

(ENERGY-068-2010) Mechanical Processing as Experimental Tool in Alternative Energy R&D (Invited)
V. P. Balema*, Sigma-Aldrich Corp., United States

4:40 PM

(ENERGY-069-2010) Microcrack Resistant Polymers Enabling Lightweight Composite Hydrogen Storage Vessels
M. Tupper*, K. Mallick, J. Cronin, P. Fabian, Composite Technology Development, Inc., United States

Nuclear

Waste Forms

Room: Dunes 1&2
Session Chair: John Marra, Savannah River National Lab

1:40 PM

(ENERGY-070-2010) Towards a Global Nuclear Renaissance: A New Paradigm for Waste Management
J. Marra*, Savannah River National Lab, United States

2:00 PM

(ENERGY-071-2010) Immobilization of Tc in a Metallic Waste Form
W. L. Ebert*, J. C. Cunnane, J. A. Fortner, Argonne National Lab, United States

2:20 PM

(ENERGY-072-2010) Fabrication and Characterization of an Alloy Waste Form for Used Nuclear Fuel
M. A. Williamson, R. L. Sindelar*, Savannah River National Laboratory, United States

2:40 PM

(ENERGY-073-2010) Characterization of a Metallic Zr-Mo Waste Form for Technetium Immobilization
E. C. Buck*, D. Gelles, J. Vienna, Pacific Northwest National Laboratory, United States

3:00 PM

(ENERGY-074-2010) Durability Testing of Glasses for the Stabilization of Closed Nuclear Fuel Cycle Waste Streams
A. L. Billings*, J. C. Marra, Savannah River National Laboratory, United States; J. V. Ryan, J. D. Vienna, J. V. Crum, Pacific Northwest National Laboratory, United States; C. S. Ray, Mo-Sci, United States

3:20 PM

Break

3:40 PM

(ENERGY-075-2010) Development of Iodine Waste Forms Using Low-Temperature Sintering Glass
T. Garino*, T. Nenoff, J. Krumhansl, D. Rademacher, Sandia National Laboratories, United States

4:00 PM

(ENERGY-076-2010) Cermet High-Level Waste Forms
R. T. Jubin*, W. S. Aaron, E. D. Collins, V. F. De Almeida, G. D. DelCul, D. W. DePaoli, L. K. Felker, B. D. Patton, S. L. Voit, Oak Ridge National Lab, United States

4:20 PM

(ENERGY-077-2010) Functionalized silica aerogels for capturing and immobilization of I, Kr, and CO2
J. Matyas*, G. E. Fryxell, K. Wallace, L. S. Fifield, Pacific Northwest National Laboratory, United States

4:40 PM

(ENERGY-078-2010) New Generation Nuclear Waste Forms Based on Nano-Encapsulation
Y. Wang*, Sandia National Laboratories, United States

Posters

Room: Horizons

7:00 PM

(ENERGY-P001-2010) Electrochemical Behaviour of Palladium Nanoparticles as Catalysts for Direct Formic Acid Fuel Cells (DFAFC)
M. Balandeh*, D. Buckley, University of Limerick, Ireland

(ENERGY-P002-2010) High Performance Nanofluids with Encapsulated Phase Change Nanoparticles for Energy Storage and Heat Transfer
Y. Hong*, W. Wu, S. Ding, L. Chow, M. Su, University of Central Florida, United States

(ENERGY-P003-2010) Fabrication and characteristics of Li-Ti-O thin film for solid state thin film supercapacitor(TFSC)
S. Kim*, Y. Yoon, Yonsei University, Korea, Republic of

(ENERGY-P004-2010) Synthesis and Characterization of Nanostructured ZnCo2O4/Co2O3 for Electrochemical Supercapacitors
O. Dominguez*, Instituto de Metalurgia UASLP, Mexico; L. M. Flores-Velez, Facultad de Quimica UASLP, Mexico; R. Cruz, Instituto de Metalurgia UASLP, Mexico; R. Martinez, I. Esparza, CIMAV, Mexico

(ENERGY-P005-2010) Advanced assessment of batteries, fuel cells & their materials using gas sorption, calorimetry and thermal analysis
A. Levchenko*, Setaram Inc, United States

(ENERGY-P006-2010) Sintered clay waste form for immobilization of cesium and strontium liquid waste
L. H. Ortega*, Texas A&M University, United States; M. D. Kaminski, Argonne National Laboratory, United States; S. M. McDeavitt, Texas A&M University, United States

(ENERGY-P007-2010) Radiation damage effects in multi-layer thin film MgO/HfO$_2$ structures
I. Usov*, J. Won, J. A. Valdez, M. Hawley, D. J. Devlin, R. M. Dickerson, G. D. Jarvinen, K. E. Sickafus, Los Alamos National Laboratory, United States

(ENERGY-P008-2010) Fabrication and Property Relations of Transuranic Actinide Containing Ceramic Oxides
S. P. Willson*, Los Alamos National Laboratory, United States

(ENERGY-P009-2010) Effects of Oxygen to Metal Ratios in High Burn-up Actinide Ceramic Oxides
J. T. Dunwoody*, S. P. Willson, D. D. Byler, K. J. McClellan, R. E. Mason, M. R. Lopez, D. R. Martinez, A. C. Martinez, Los Alamos National Laboratory, United States

(ENERGY-P010-2010) Utilization of Pondash in Highway Engineering
R. Sarkar, A. Varma*, A. Garg, M. Saxena, P. Sharma, N. Khanna, Delhi College of Engineering, India

(ENERGY-P011-2010) The performances of ceramic based membranes for fuel cells
U. Thanganathan*, Okayama University, Japan

(ENERGY-P012-2010) Kinetics of H2 Desorption from TiN-Destabilized NaAlH4
W. D. Ukpai*, S. Narase Gowda, T. A. Dobbins, Louisiana Tech University, United States

(ENERGY-P013-2010) Empirical Method to Estimate Hydrogen Embrittlement of Metals as a Function of Hydrogen Gas Pressure at Constant Temperature
J. A. Lee*, NASA-Marshall Space Flight Center, United States

(ENERGY-P014-2010) Ultrasmall Angle X-ray Scattering (USAXS) Studies of Mophological Changes in NaAlH4
S. Narase Gowda*, T. A. Dobbins, Louisiana Tech University, United States

(ENERGY-P015-2010) Ammonium borohydride: Solid Hydrogen Storage Material with Highest Gravimetric Hydrogen Content
A. Karkamkar*, D. Heldebrant, J. Linehan, T. Autrey, Pacific Northwest National Lab, United States

(ENERGY-P016-2010) Performance Evaluation of Oxide Catalyst-doped Ni-Zirconia and Ni-Ceria based Anodes for Methane Fueled SOFCs
J. Myung*, J. Lee, S. Hyun, Yonsei University, Korea, Republic of

(ENERGY-P017-2010) Carbon Building Materials from Coal Char: Durable Materials for Solid Carbon Sequestration
J. Halloran*, University of Michigan, United States

(ENERGY-P018-2010) Environmental Catalysts from Biochar
J. Kastner*, University of Georgia, United States; P. Kolar, North Carolina State University, United States; A. Teja, Georgia Tech, United States

(ENERGY-P019-2010) Superhydrophobic membrane distillation for water desalination
M. Su, University of Central Florida, United States; Z. Ma*, Y. Hong, L. Ma, Unversity of Central Florida, United States

(ENERGY-P020-2010) On enhancing efficiency of dye-sensitized solar cells by MPII-implanted ruthenium ions
D. Wang, MingDao University, Taiwan; C. Yen*, National Chung Hsing University, Taiwan; M. Shih, MingDao University, Taiwan; L. Chang, National Chung Hsing University, Taiwan; H. Shih, Chinese Culture University, Taiwan

(ENERGY-P021-2010) Spin-engineered suppression of dominant non-radiative shunt paths in Ga(In)NAs relevant to photovoltaic applications
X. J. Wang, Y. Puttisong, Linköping University, Sweden; C. W. Tu, University of California, United States; A. J. Ptak, National Renewable Energy Laboratory, United States; V. K. Kalevich, A. Y. Egorov, A F Ioffe Physico-Technical Institute, Russian Federation; L. Geelhaar, H. Riechert, Paul-Drude-Institut für Festkörpelektronik, Germany; I. A. Buyanova, W. M. Chen*, Linköping University, Sweden

(ENERGY-P022-2010) The Potential of Fiber Optimization for Transport of Solar Radiations
J. Wang*, National Sun Yat-Sen University, Taiwan

(ENERGY-P023-2010) Cu2ZnSnSe4 thin films produced by selenization of Cu-Zn-Sn containing precursor films
O. Volobujeva*, E. Mellikov, S. Bereznev, J. Raudoja, Tallinn University of Technology, Estonia

(ENERGY-P024-2010) Mechanical and Rheological Properties of Blends of Poly (phenylene sulfide) and Liquid Crystalline Polymers: The use of Recycled Poly (ethylene terephthalate)
H. Shaban*, Kuwait University, Kuwait

Wednesday, February 24, 2010

Hydrogen

Nanostructures and Catalytic Materials for Hydrogen Storage

Room: Seashore Ballroom

Session Chairs: Rana Mohtadi, Toyota Research Institute of North America; Gavin Walker, University of Nottingham

8:00 AM

(ENERGY-079-2010) Savannah River National Laboratory Regenerative Fuel Cell Project
T. Motyka*, Savannah River National Laboratory, United States

8:20 AM

(ENERGY-080-2010) Novel high temperature proton conducting polymer electrolyte membrane
J. Iroh*, W. Lu, J. Wang, University of Cincinnati, United States

8:40 AM

(ENERGY-081-2010) Fabrication of Palladium Coated Nanoporous Carbon Nanofibers via Electrospinning
H. Kim*, Yonsei University, Korea, Republic of; D. Lee, Yonsei University, Korea, Republic of; J. Moon, Yonsei University, Korea, Republic of

9:00 AM

(ENERGY-082-2010) Nanostructured Platinum for Fuel Cells
F. van Swol*, Y. Song, M. A. Hickner, Sandia National Laboratories, United States; S. R. Challa, R. M. Garcia, H. Wang, C. J. Medforth, University of New Mexico, United States; J. E. Miller, J. A. Shelnutt, Sandia National Laboratories, United States

9:20 AM

(ENERGY-083-2010) Novel Hydrogen Storage Properties Derived from Nanoscale LiBH4 (Invited)
L. Shaw*, X. Wan, Y. Zhong, K. Crosby, University of Connecticut, United States

9:40 AM

(ENERGY-084-2010) Environmentally benign palladium membrane reactor for hydrogen production (Invited)
Y. H. Ma*, Worcester Polytechnic Institute, United States

10:00 AM

Break

10:20 AM

(ENERGY-085-2010) Nano-materials for Hydrogen Storage (Invited)
P. Jena*, Virginia Commonwealth University, United States

10:40 AM

(ENERGY-086-2010) Novel Carbon Nanostructures Composites for Hydrogen Storage
R. Zidan*, M. A. Wellons, J. Teprovich, Savannah River National Laboratory, United States

11:00 AM

(ENERGY-087-2010) Metal-Assisted Hydrogen Uptake on Nanoporous Carbon Materials (Invited)
C. Contescu*, V. V. Bhat, N. C. Gallego, Oak Ridge National Laboratory, United States

11:20 AM

(ENERGY-088-2010) Dynamics of hydrogen adsorption on graphene and silicene: Ab initio computer simulations (Invited)
A. Farajian*, Wright State University, United States

11:40 AM

(ENERGY-089-2010) The potential role of Mg-based hydrides for the improvement of negatives electrodes for advanced batteries (Invited)
M. Latroche*, ICMPE UMR7182 CNRS, France

Battery Technology

Energy Storage and Conversion II

Room: Sawgrass

Session Chair: Gene Kim, Cookson Electronics Assembly Materials Group

8:00 AM

(ENERGY-090-2010) High Energy Density Metal Oxide Anodes for Li-ion Batteries (Invited)
A. C. Dillon*, C. Ban, L. A. Riley, Z. Wu, D. T. Gillaspie, National Renewable Energy Laboratory, United States; L. Chen, Y. Yan, S. Lee, University of Colorado at Boulder, United States

8:40 AM

(ENERGY-091-2010) Electrochemical performance of metal oxide coated LiNi0.5Mn1.5O4 material
A. Abouimrane*, H. Wu, I. Belharouak, K. Amine, Argonne National Laboratory, United States

9:00 AM

(ENERGY-092-2010) Lithium Accumulator Capacity Increase via Three-Dimensional Construction of Electrodes
J. Prochazka*, L. Kavan, M. Zukalova, JHI, Czech Republic

9:20 AM

(ENERGY-093-2010) Structure and Electrochemistry of Li2MnSiO4 Cathode Material
I. Belharouak*, A. Abouimrane, K. Amine, Argonne National Laboratory, United States

9:40 AM

(ENERGY-094-2010) CZTS Monograin Materials for Photovoltaics
E. Mellikov*, Tallinn University of Technology, Estonia; D. Meissner, Crystalsol OÜ, Estonia; M. Altosaar, J. Raudoja, K. Timmo, T. Varema, M. Kauk, J. Krustok, O. Volobujeva, M. Danilson, Tallinn University of Technology, Estonia; K. Muska, T. Badegruber, W. Ressler, K. Ernits, F. Lehner, Crystalsol OÜ, Estonia

10:00 AM

Break

10:20 AM

(ENERGY-095-2010) Lithium Storage Characteristics in Nano Graphene Platelets–based Materials (Invited)
C. Strope, T. Pham, H. Huang*, Wright State University, United States

11:00 AM

(ENERGY-096-2010) In-situ Impedance Measurements of LiMn1.5Ni0.4Cr0.1O4 Cathode During Charge/Discharge Cycling
K. Asmar, R. Singhal, R. S. Katiyar, University of Puerto Rico, Rio Piedras, Puerto Rico; A. Sakla, H. Abernathy, A. Manivannan*, US DOE, National Energy Technology Laboratoty, United States

11:20 AM

(ENERGY-097-2010) Optimization of LixNi0.25CoyMn0.75-yO2±θ (x=1.225-1.65, y=0, 0.15) for High Energy Battery Applications
H. Deng*, I. Belharouak, H. Wu, K. Amine, Argonne National Lboratory, United States

11:40 AM

(ENERGY-098-2010) Rapid Synthesis of Electrode Materials (Li4Ti5O12 and LiFePO4) for Lithium Ion Batteries Through Microwave Enhanced Processing Techniques
K. Cherian*, M. Kirksey, Spheric Technologies Inc, United States; A. Kasik, M. Armenta, S. Dey, Arizona State University, United States

Biomass

Materials Compatibilty with Biofuels

Room: Dunes 1&2

Session Chair: Edgar Lara-Curzio, Oak Ridge National Laboratory

8:00 AM

(ENERGY-099-2010) Addressing the Materials Challenges in Converting Biomass to Energy
C. Powell*, J. Bennett, B. Morreale, National Energy Technology Laboratory, United States

8:20 AM

(ENERGY-100-2010) An Aggregation of Materials Composition Studies for Fuel Ethanol (Invited)
K. Moore*, Renewable Fuels Association, United States

8:40 AM

(ENERGY-101-2010) Overview of Materials Compatibility Issues with Fuel Grade Ethanol (Invited)
J. Beavers*, F. Gui, DNV Columbus, Inc., United States; A. Ertekin, N. Sridhar, DNV Research and Innovation, United States

9:00 AM

(ENERGY-102-2010) Compatibility Assessment of Fuel Dispenser Metals and Elastomers in an Aggressive E20 Fuel
M. Kass, S. Pawel, C. Janke, T. Theiss, S. Lewis, Oak Ridge National Lab, United States; W. Clark, National Renewable Energy Laboratory, United States; J. Chapin*, K. Boyce, T. Fabian, J. Bablo, Underwriters Laboratories, Inc., United States

9:20 AM

(ENERGY-103-2010) Microturbines and Biomass Fuels – Materials Challenges
W. Matthews*, Capstone Turbine Corporation, United States; K. More, L. Walker, Oak Ridge National Laboratory, United States

9:40 AM

(ENERGY-104-2010) Material Characterization and Analysis for Selection of Refractories Used In Black Liquor Gasification
J. G. Hemrick*, J. R. Keiser, R. A. Peascoe-Meisner, Oak Ridge National Laboratory, United States

10:00 AM

Break

10:20 AM

(ENERGY-105-2010) Performance of Materials in Biomass Gasification systems
J. R. Keiser*, P. J. Blau, B. A. Pint, Oak Ridge National Laboratory, United States; R. A. Meisner, University of Tennessee-Knoxville, United States; J. G. Hemrick, Oak Ridge National Laboratory, United States

10:40 AM

(ENERGY-106-2010) Volatility of Inorganics During the Gasification of Dried Sludge
C. Bourgel*, J. Poirier, CNRS-CEMHTI, France; F. Defoort, J. Seiler, CEA/DTN/SE2T/LTE, France; C. Peregrina, Material recycling and energy recovery Division, CIRSEE, France

11:00 AM

(ENERGY-107-2010) Catalysts and Sorbents for Thermochemical Conversion of Biomass—Material Development Needs
S. Cheah*, K. Magrini-Bair, National Renewable Energy Laboratory, United States

11:20 AM

(ENERGY-108-2010) Air Force Research Lab Bio Technology (Invited)
O. Mendoza*, Air Force Research Lab, United States

11:40 AM

(ENERGY-109-2010) Solid Catalysts from Biochar
J. Kastner*, D. Geller, J. Miller, University of Georgia, United States; L. Keith, Down to Earth Energy, LLC, United States

Wind

Materials Trends and Opportunities for Wind Energy Applications

Room: Sea Oats

Session Chairs: Tom Ashwill, Sandia; Douglas Cairns, Montana State University

8:00 AM

(ENERGY-110-2010) Selection of Wind Turbine Blade Materials for Fatigue Resistance
J. F. Mandell*, Montana State University, United States

8:20 AM

(ENERGY-111-2010) Materials Solutions for Wind Energy (Invited)
P. J. Dougherty*, SMI Inc./Helios Strategies, United States

8:40 AM

(ENERGY-112-2010) Advanced Composite Materials and Manufacturing Processes Increase Wind Turbine Size and Reliability
M. Tupper*, M. Hulse, J. Cronin, W. Francis, K. Mallick, CTD, United States

9:00 AM

(ENERGY-113-2010) Materials Challenges and Opportunities in Wind Energy (Invited)
F. D. Marquis*, Naval Postgraduate School, United States

9:20 AM

(ENERGY-114-2010) Effects of Fiber/Matrix ratios and Dry and Wet Environments on the Mechanical Properties of Carbon/Polyurethane Composites
M. Farooq*, C. Lazzara, J. Bicerano, P. Viens, Neptune Research Inc., United States

9:40 AM

Break

10:00 AM

(ENERGY-115-2010) Embedded Sensors for Composite Wind Turbine Blades
D. Cairns*, Montana State University, United States

10:20 AM

(ENERGY-116-2010) Printed Sensors for System State of Health Monitoring
P. Clem*, C. A. Apblett, E. D. Branson, J. F. Carroll, K. R. Fenton, Sandia National Laboratories, United States

10:40 AM

(ENERGY-117-2010) Development of Multifunctional Nanocomposite Coatings for Wind Turbine Blades
J. Gou*, Y. Tang, F. Liang, J. Kapat, University of Central Florida, United States

11:00 AM

(ENERGY-118-2010) Novel cost-effective materials and processes for Wind Energy
A. Kumar*, Z. Liang, B. Wang, C. Zhang, O. Okoli, T. Liu, C. Zeng, A. Vanli, M. Zhang, HPMI, Florida State University, United States

11:20 AM

(ENERGY-119-2010) Nanostrength® Block Copolymers for Wind Energy
R. Barsotti*, J. Chen, A. Alu, Arkema, Inc, United States

Hydrogen

Characterization and Analysis of Hydrogen Storage Materials

Room: Seashore Ballroom

Session Chairs: Ashley Stowe, B&W Y-12 National Security Enterprise; Sonjong Hwang, Californina Institute of Technology

1:40 PM

(ENERGY-120-2010) Characterization Studies of Boron-Containing Compounds for Hydrogen Storage Applications (Invited)
R. C. Bowman*, Oak Ridge National Laboratory, United States; S. Hwang, C. Kim, California Institute of Technology, United States; G. M. Brown, D. A. Knight, Oak Ridge National Laboratory, United States; J. Zhao, The Ohio State University, United States; J. W. Reiter, J. A. Zan, Jet Propulsion Laboratory, United States; G. L. Soloveichik, S. Kniajanski, GE Global Research, United States

2:00 PM

(ENERGY-121-2010) Multinuclear High Resolution Solid State NMR studies of Dodecaborate Intermediate of Borohydrides based Hydrogen Storage Systems
S. Hwang*, C. Ahn, J. W. Reiter, J. A. Zan, California Institute of Technology, United States; V. Stavila, Sandia National Laboratories, United States; J. J. Vajo, HRL Laboratories, LLC, United States

2:20 PM

(ENERGY-122-2010) Contributions from anelastic spectroscopy to the study of complex hydrides (Invited)
R. Cantelli*, Sapienza University of Rome, Italy; A. Paolone, CNR-INFM Laboratorio Regionale Supermat, Italy; O. Palumbo, ISC-CNR Istituto dei Sistemi Complessi, Italy; P. Rispoli, Sapienza University of Rome, Italy

2:40 PM

(ENERGY-123-2010) New Possibilities for Understanding Complex Metal Hydrides via Synchrotron X-ray Studies
T. A. Dobbins*, Louisiana Tech University, United States

3:00 PM

(ENERGY-124-2010) Structural study and hydrogen sorption kinetics of ball-milled samples of cast Mg-10%Ni catalysed by Nb
S. Aminorroaya-Yamini*, A. Ranjbar, H. K. Liu, University of Wollongong, Australia; Y. Cho, A. K. Dahle, University of Queensland, Australia

3:20 PM

Break

3:40 PM

(ENERGY-125-2010) Recent Results from DOE's Chemical Hydrogen Storage Center of Excellence (Invited)
K. Ott*, Los Alamos National Lab, United States

4:00 PM

(ENERGY-126-2010) In-situ neutron diffraction for characterization of hydrogen storage and infrastructure materials (Invited)
L. Laversenne*, L. Cagnon, P. De Rango, D. Fruchart, CNRS Institut Neel, France; J. Huot, IRH-Universite du Quebec a Trois-Rivieres, Canada; S. Miraglia, V. Nassif, CNRS Institut Neel, France; S. F. Santos, IRH-Universite du Quebec a Trois-Rivieres, Canada; N. Skryabina, Perm State University, Russian Federation

4:20 PM

(ENERGY-127-2010) Analysis of Cryosorption System for Hydrogen Storage (Invited)
R. Chahine*, HRI - Universite du Quebec a Trois-Rivieres, Canada

4:40 PM

(ENERGY-128-2010) Analysis of Thermal Decomposition of t-Butylamine Borane (Invited)
A. C. Stowe*, N. Smyrl, J. Morrell, J. Feigerle, B&W Y-12 National Security Enterprise, United States

Battery Technology

Energy Storage and Conversion III

Room: Sawgrass

Session Chairs: Vijay Jain, URS Washington Division; Joshua Gray, Savannah River National Laboratory

1:40 PM

(ENERGY-129-2010) HeteroFoaMs: A New Frontier in Energy Storage and Conversion Materials
K. Reifsnider*, F. Rabbi, Univ. of South Carolina, United States

2:00 PM

(ENERGY-130-2010) Development of Nano/Micro-structured Materials for Energy Storage (Invited)
H. Cheng*, Chinese Academy of Sciences, China

2:20 PM

(ENERGY-131-2010) Development of Advanced Low-Temperature Sodium-Beta Alumina Batteries
X. Lu*, G. Xia, K. Meinhardt, J. Lemmon, V. Sprenkle, Z. Yang, Pacific Northwest National Laboratory, United States

2:40 PM

(ENERGY-132-2010) Ionogels as Solid Electrolytes for Advanced Battery Applications
J. Gray*, H. Colon-Mercado, B. Garcia-Diaz, A. Visser, M. Williamson, M. Au, T. Adams, Savannah River National Laboratory, United States

3:00 PM

(ENERGY-133-2010) Quantitative Characterization of Lithium Ion Batteries by Microscopic Techniques
T. Bernthaler, C. N. Hafner*, R. Löffler, A. Nagel, V. Pusch, G. Schneider, Hochschule Aalen, Germany

3:20 PM

Break

3:40 PM

(ENERGY-134-2010) Microstructural Control and Characterization of BICUVOX Ceramics
S. Razmyar*, K. Sabolsky, E. M. Sabolsky, West Virginia University, United States

4:20 PM

(ENERGY-135-2010) Texture Development during Hot Deformation of Bismuth Telluride and Bismuth Telluride based Composites (Invited)
R. Srinivasan*, Wright State University, United States; N. Gothard, J. Spowart, Air Force Research Laboratory, United States

Nuclear

Modeling and Simulation

Room: Dunes 1&2

Session Chairs: Alex Larzelere, U.S. Department of Energy; Marius Stan, Los Alamos National Laboratory

1:40 PM

(ENERGY-136-2010) Nuclear Energy Advanced Modeling and Simulation: An Introduction (Invited)
A. Larzelere*, U.S. Department of Energy, United States

2:00 PM

(ENERGY-137-2010) Advanced Models and Simulations of Nuclear Fuels (Invited)
M. Stan*, Los Alamos National Laboratory, United States

2:20 PM

(ENERGY-138-2010) Center for Materials at Irradiation and Mechanical Extremes (Invited)
M. Nastasi*, Los Alamos National Laboratory, United States

2:40 PM

(ENERGY-139-2010) Defect Dynamics of Irradiated Microstructures (Invited)
T. Arsenlis*, M. Rhee, G. Hommes, Lawrence Livermore National Laboratory, United States

3:00 PM

(ENERGY-140-2010) A Perspective on Mesoscale Modeling of Irradiated Nuclear Reactor Materials (Invited)
A. El-Azab*, Florida State University, United States

3:20 PM

Break

3:40 PM

(ENERGY-141-2010) Fission Gas Behavior in UO_2: Atomistic Simulation of Multidimensional Defects
C. Stanek*, D. Andersson, B. Uberuaga, P. Nerikar, Los Alamos National Laboratory, United States

4:00 PM

(ENERGY-142-2010) Activation energies for Xe transport in $UO_{2\pm x}$ from density functional theory calculations
D. Andersson*, P. Nerikar, B. Uberuaga, C. Stanek, Los Alamos National Laboratory, United States

Hydropower

Materials Challenges in Hydro and Geothermal Energy

Room: Sea Oats

Session Chairs: Brenda Garcia-Diaz, Savannah River National Laboratory; Hidda Thorsteinsson, U.S. Dept. of Energy

1:40 PM

(ENERGY-143-2010) Ocean Thermal Energy Conversion: Heat Exchanger Evaluation and Selection (Invited)
M. A. Laboy*, Offshore Infrastructure Associates, Puerto Rico; O. E. Ruiz, University of Puerto Rico - Mayaguez Campus, Puerto Rico; J. Martí, Technical Consulting Group, Puerto Rico

2:00 PM

(ENERGY-144-2010) Optimal Operation of Cascaded Hydroelectric Plants in Energy Market with Considering Value of Water (Invited)
M. Heidarizadeh*, M. Aghamohammadi, power and water university of Technology, Iran, Islamic Republic of; T. Akbari, tehran university, Iran, Islamic Republic of; M. Ahmadian, power and water university of Technology, Iran, Islamic Republic of

2:20 PM

(ENERGY-145-2010) Advanced Composite Materials for Tidal Turbine Blades
M. Tupper*, M. Hulse, J. Cronin, W. Francis, CTD, United States

2:40 PM

(ENERGY-146-2010) Effect of delta ferrite on impact properties of low carbon 13Cr4Ni martensitic stainless steel
P. Wang*, S. Lu, N. Xiao, D. Li, Y. Li, Institute of Metal Research,Chinese Academy of Sciences, China

3:00 PM

(ENERGY-147-2010) Martensitic Stainless Steel 0Cr13Ni4Mo for Hydraulic Runner (Invited)
Y. Li*, D. Li, Institute of metal research, Chinese Academy of Sciences, China

3:20 PM

Break

3:40 PM

(ENERGY-148-2010) Alloy Testing, Selection, and Condition Monitoring Challenges for Geothermal Energy Systems
B. Amend*, DNV Columbus, Inc., United States

4:00 PM

(ENERGY-149-2010) Experience with the Development of Advanced Materials for Geothermal Systems
T. Sugama, T. Butcher*, Brookhaven National Laboratory, United States

4:20 PM

(ENERGY-150-2010) Novel High Temperature Materials Enabling Operation of Equipment in Engineered Geothermal System Wells
M. Tupper*, C. Hazelton, M. Hooker, K. Kano, L. Adams, Composite Technology Development, Inc., United States

Monday, February 22, 2010

Tutorial Session

Room: SeaOats/Sawgrass/Dunes 1&2

8:30 AM

(ENERGY-001-2010) Advances in Battery Technology (Invited)

Y. Chiang*, Massachusetts Institute of Technology, United States

Abstract not available

9:15 AM

(ENERGY-002-2010) Achievements and Perspectives of the US National Program on Hydrogen Storage (Invited)

N. T. Stetson*, C. Read, S. Dillich, G. Ordaz, M. Gardiner, R. Bowman, U.S. Department of Energy, United States

The U.S. DOE Hydrogen Program's mission is to reduce oil use and carbon emissions and to enable clean, reliable energy for stationary, portable power generation and transportation. The requirements for hydrogen storage continue to be some of the most technically challenging barriers to the widespread commercialization of hydrogen fuel cell products. The DOE-EERE hydrogen storage activities primarily focus on applied research and development of materials and engineering to provide low-pressure storage options that meet packaging, cost, safety and performance requirements to allow fuel cell systems to be competitive with current technologies. This presentation summarizes the status, recent accomplishments and current performance gaps of hydrogen storage technologies for fuel cell applications. The research is conducted under the framework of DOE's National Hydrogen Storage Project that includes independent projects and Centers of Excellence in both applied and basic hydrogen storage R&D. Material projects are focused in three main areas: metal hydrides; chemical hydrogen storage materials and hydrogen sorbents. There are several new efforts, including the Hydrogen Storage Engineering Center of Excellence, which will provide a coordinated approach to engineering research and development of hydrogen storage systems.

10:15 AM

(ENERGY-003-2010) Photovoltaics: Past, Present, and Future (Invited)

R. P. Raffaelle*, National Renewable Energy Lab, United States

This tutorial will summarize the current landscape concerning photovoltaic development, demonstration, and deployment. A review of the basic cell types and the current benchmarks for performance will be given. A particular focus will be placed on the materials challenges and opportunities pertaining to the various conversion technologies being pursued. An overview of the current photovoltaics market and the impact that various national and international deployment programs have had on its development will be convered. Finally, next-generation approaches to photovoltaic conversion and their prospects for the future of the field will be discussed.

11:00 AM

(ENERGY-004-2010) Wind Energy: Background, Technology Opportunities, and Material Challenges (Invited)

J. Zayas*, Sandia National Laboratories, United States

Wind Energy is one of the fastest-growing sources of utility-scale power generation in the US today, representing nearly 40% of the total new capacity added in 2008 (second only to natural gas). Through the 3rd quarter of 2009, wind power provides approximately 31GW of the electricity generating capacity in the U.S, or just over 2.0% of the nation's electricity. As the technology continues to move forward, increases in efficiency, performance, and reliability must continue to be in the forefront of the research activities that will facilitate the sustained growth of the industry. This presentation will outline the history of the technology, the trends and challenges faced by the industry, and describe the ongoing and future technical research activities that are targeted at enhancing current wind generation.

11:45 AM

(ENERGY-005-2010) Materials Challenges in Nuclear Energy (Invited)

S. J. Zinkle*, Oak Ridge National Laboratory, United States

Nuclear power currently provides 20% of the US electricity via 104 operating nuclear power plants, and about 30 new reactors may begin construction in the US during the next ten years. These new reactors would be based on evolutionary 3rd generation (Gen III) nuclear technology, which utilizes water as the coolant with a typical operating temperature near 330°C. This technology is similar to existing Gen II nuclear power plants that have recent capacity factors exceeding 90% in the US. There is also growing interest in so-called Gen IV concepts that would increase thermodynamic efficiency via higher operating temperatures. The successful implementation of these next generation nuclear power systems is directly linked with development of high-performance materials. For Gen III reactors, key issues include 1) continued improvements in water chemistry control and steam generator materials with extreme resistance to aqueous stress corrosion cracking, 2) development of new cladding materials that will reliably enable higher fuel burnup levels, and 3) use of radiation damage-resistant materials in the reactor internal structures to enable very long reactor lifetimes (60 years and beyond). For Gen IV reactors, key issues include 1) development of structural materials capable of operating at very high temperatures and neutron damage levels in the presence of diverse coolants such as liquid sodium and gaseous helium, 2) development of new fuel systems, and 3) development of materials for reliable and high-efficiency electricity production and high temperature process heat applications such as hydrogen production. This presentation will provide an overview of materials research and development issues that require solutions to enable the next series of power reactors (Gen III and Gen IV) to operate with the highest levels of efficiency and safety.

2:15 PM

(ENERGY-006-2010) Material Needs in Alternative and Renewable Energy for the Automotive Industry (Invited)

M. Verbrugge*, GM R&D, United States

The first portion of this talk will relate global energy challenges to trends in personal transportation. Following this introduction, a short overview of promising automotive traction technologies will be discussed, including GM programs aimed at the deployment of vehicles based on the enabling technologies: alternative fuel vehicles, extended-range electric vehicles (EREVs), and fuel cell vehicles (FCEVs). The final portion of this talk will highlight the progress and challenges associated specifically with lithium ion batteries, consistent with the imminent large-scale use of lithium ion batteries for traction applications.

3:00 PM

(ENERGY-007-2010) Striking a Balance to Allow the Defense Industry to Fully Participate in Meeting Alternative and Renewable Energy Goals (Invited)

K. Billings*, Lockheed Martin, United States

Much is made of the perceived evils of the so called "revolving door" between government and the private sector. In 1961 when President Eisenhower warned of the Military Industrial Complex in his farewell address, he also spoke of the important role of industry in providing the necessary the technology and the advancements that would be necessary to keep the world free and sustain the American way of life. His emphasis was not so much of the dangers of the Military Industrial Complex, but the need for balance. A fresh perspective is needed to be brought to that balance, especially as it relates to meeting our nation's and the world's energy and climate challenges.

4:00 PM

(ENERGY-008-2010) Air Force Energy Strategy (Invited)

G. Wright*, AFRL, United States

This presentation will provide a brief overview of the Air Force Energy Strategy. The Air Force Energy Strategy supports the creation of a National Energy Strategy. Specifics will be given detailing the Air Force energy vision and its supporting three-pronged energy strategy.

4:45 PM

(ENERGY-009-2010) Advanced Materials for Our Energy Future: Study Results (Invited)

S. DeVincent Wolf*, Materials Research Society, United States; D. Dimos, Sandia National Laboratories, United States

A study has been conducted to highlight materials research needs for meeting the global energy and climate challenges and is the result of a collaborative effort of numerous professional societies representing the materials research community. The primary outcome of this study is a report for communicating with policy leaders in Washington D.C. as well as being an easy to understand reference for the media, schools, etc. The report showcases success stories that have resulted from investment in materials research and focuses on key areas of needed investment where breakthroughs in materials research can have a significant impact. This report is meant to complement recent studies of science and technology needs for energy, by focusing on the role of materials technologies in energy efficiency, energy supply, protection of the environment and job creation.

Tuesday, February 23, 2010

Solar

Coating and Silicon Based PVs

Room: Sea Oats

Session Chair: Abhi Karkamkar, Pacific Northwest National Lab

8:00 AM

(ENERGY-010-2010) Silicone Materials for Photovoltaic Module Assembly

A. Norris*, M. Tomalia, B. Ketola, Dow Corning Corporation, United States

Silicone polymers have key material properties that make them excellent candidates for many applications in photovoltaic module assembly. These advantages included excellent UV stability, corrosion resistance, low moisture retention, wide temperature use range and excellent electrical properties. Due to their low modulus and low glass transition temperature, silicones are recognized for their stress-relieving characteristics over a wide temperature range. Silicones have been proven to have higher transparency resulting in increased module efficiency and improved durability than current organic materials used in PV encapsulation. These improvements transparency and durability both contribute to and are key to the overall PV industry goal of decreasing the $/kWh. As the photovoltaic industry expands, it is critical to select suitable material and process solutions to meet the numerous requirements including durability, performance, cost, throughput and global availability. This review will focus on the unique properties of silicones that make them ideal products for the entire PV module assembly market including encapsulation, frame sealant, and junction box potting.

8:20 AM

(ENERGY-011-2010) Biomimetic Nanostructured Anti-Reflection Coatings for Highly Efficient Solar Cells

M. Kane*, Savannah River National Laboratory, United States; P. Jiang, University of Florida, United States

Solar energy is clean, abundant, and renewable, yet vastly under-utilized due to the high manufacturing and installation costs of photovoltaics. Current production of solar cells is dominated by crystalline silicon modules; however, due to the high refractive index of silicon, more than 35% of incident light is reflected. Various antireflection coatings (ARCs) have been developed to reduce reflective losses but high manufacturing costs and limited performance have impeded development of solar cells that can be made competitive with fossil fuels. Nanostructured moth-eye anti-reflection coatings were developed to highly reduce the reflections from both the silicon surface and glass encapsulation layer. These ARCs were produced by a robust templating nanofabrication technique that combines the simplicity and cost benefits of bottom-up self-assembly with the scalability and compatibility of top-down microfabrication. In this study, the structure property relationship of these coatings and environmental stability were characterized in order to advance this technology for terrestrial and space-based solar applications. The geometry of the biomimetic nanostructured ARC was optimized for maximum solar cell efficiency and the environmental tolerance of the ARC was tested by accelerated and long term material aging studies, including stability in heat, moisture, and ionizing radiation environments.

8:40 AM

(ENERGY-012-2010) Novel Resilient Flux Coated ReadyRibbonTM Solder Ribbon for Polysilicon Photovoltaic Cell Module Assembly

G. Kim*, M. Marczi, G. Cunning, O. Khaselev, Cookson Electronics Assembly Materials Group, United States

This presentation will introduce a novel solder-coated ribbon used in the interconnection of polysilicon photovoltaic module assembly. The resilient flux technology used in the ReadyRibbonTM allows for (1) better manufacturing process control through the elimination of process and maintenance steps involved with liquid flux application, (2) improved reliability through the uniformity of the resilient flux, and (3) increased efficiency of the photovoltaic cells through better quality of the interconnect.

9:00 AM

(ENERGY-013-2010) Vapor-liquid-solid grown silicon nanowire solar cells

J. Greil*, A. Lugstein, E. Bertagnolli, Vienna University of Technology, Austria

We present synthesis and characterization of thin film silicon solar cells utilizing silicon nanowires as building blocks. Radial p-n junction devices were suggested to have potential advantages over planar geometries due to orthogonalization of charge carrier seperation and drift transport. Arrays of epitaxially grown silicon nanowires were synthesized via the Vapor-Liquid-Solid process and coated with polycrystalline silicon. Base and emitter doping was performed according to a proximity rapid thermal diffusion technique in a two step process (pre-deposition and drive-in) allowing for well controlled dopant concentration. SEM analysis of the poly-Si layer shows uniform coverage along the nanowire length and reveals the polycrystalline structure of the film. The bottom-up synthesis process allows the rational control of device structure, size and morphology. Utilization of an ex-situ doping technique enables uniform base dopant concentration and a controllable emitter doping profile. We recognize the importance of well controlled film deposition and doping conditions. The impact of varying these conditions on the efficiency of the solar cell was investigated and an optimized device is presented.

9:20 AM

(ENERGY-014-2010) Synthesis of Solar-grade Silicon from Amorphous Silica (Rice Husk Ash)

K. K. Larbi*, M. Barati, A. McLean, R. Roy, University of Toronto, Canada

Impurity optimized silicon is needed for the advancement of terrestrial photovoltaic power generation. In this study an approach to synthesis of solar grade silicon using rice husk ash has been pursued. Metallothermic reduction of the purified rice husk ash was investigated within the temperature range of 500-950 C using magnesium in varied amounts. The reduction product was purified by two stage acid leaching sequence. Analysis of the final silicon product by XRD, SEM, and ICP-OES showed crystalline silicon with B and P content to be less than 3 ppm and 72 ppm respectively. Transitional metal impurities and other elements were all reduced in various processing steps. Based on the results it can be concluded that rice husk ash is a promising starting material for production of solar grade silicon.

9:40 AM

(ENERGY-015-2010) Rice Hulls to Solar Grade Silicon

M. Mede*, Thermal Technology LLC, United States; P. Italiano, Costech International s.P.a., Italy; S. Cooke, Solution Research, United States

Thermal Technology,LLC of California and Costech International s.P.a.of Italy have teamed to develop a new process for the production of Solar Grade Silicon using the by product of rice production, the rice hull. The new process is the first to combine pyrolysis with carbo thermic reduction yielding an integrated, energy and cost effect method for the production of solar grade silicon. The process utilizies pyrolysis to produce the suitable blend of SiO2 and C while providing direct electrical energy which is connected to carbo thermic reduction furnaces. Pyrolyized material is cleaned and fed into the reduction furnaces which casts silicon into molds suitable for sale to crystal growers or poly crystaline wafer producers. The paper discusses the process, energy consumption, comparisons to current industrial processes and final product properties.

10:20 AM

(ENERGY-016-2010) Metallurgical Refining of Silicon for Solar Applications by Slagging of Impurity Elements

M. Johnston*, M. Barati, University of Toronto, Canada

New measurements have been made on the distribution of impurity elements between molten metallurgical silicon and slags of the type Al_2O_3-CaO-MgO-SiO_2 and CaF_2-CaO-SiO_2. Distribution coefficients were determined for Al, B, Ca, Mg, Fe and P between magnesia or alumina saturated slags and silicon at 1500 °C. The partitioning behaviour of the impurity elements between the molten phases was examined in terms of the basicity of the fluoride-containing slag and both the basicity and the oxidising characteristics of the oxide slag. Experiments were also conducted to determine the effect of oxygen partial pressure on the partitioning of the impurity elements. The data were used to generate fundamental thermodynamic values relevant to silicon purification with the aim of producing PV grade silicon.

10:40 AM

(ENERGY-017-2010) A Novel Purification Method for Production of Solar Grade Silicon

S. Esfahani*, M. Barati, Z. Yin, University of Toronto, Canada

Purification of metallurgical grade silicon (MG- Si) by a combination of solvent refining and physical separation has been studied. MG-Si was alloyed with iron and solidified with different cooling rates to grow pure Si dendrites from the alloy. The Si dendrites and FeSi2 that were formed after solidification were then separated by a gravity-based method, using heavy media. Since pure Si particles have much less density than FeSi2, they formed a thick layer on the top of heavy media and the FeSi2 particles were settled at the bottom. The effect of particle size and cooling rate on the yield and separation efficiency of the Si phase was investigated. The floated Si particles were further purified by removing the physically adherent Fe-Si phase, using an acid leaching method. Analysis of the produced silicon indicates that several impurity elements can be efficiently removed using this simple and low-cost technique.

11:00 AM

(ENERGY-018-2010) Thermal heat storage in inorganic molten salt slurries for solar central electricity

M. Zare*, R. Abbaschian, University of California, Riverside, United States

Inorganic molten salts are of considerable interest for thermal energy storage due to their high storage capacity for sensible or latent heat during a phase change. The latter techniques provides much higher energy storage density than the former, thus enabling more efficient subsequent conversion of the stored energy to electrical energy. However, the major issues are related to the difficulties of heat transfer between heat exchanger system and PCM, and volume change during the phase transformation. An approach to deal with those is to circulate solid-liquid PCM slurry, for which the energy storage is achieved by changing the fraction solid during the thermal cycling. In this study, the feasibility of using various inorganic salt mixtures for thermal storage in the solar central power plant have been investigated, and a screening methodology for the selection of salt mixtures and compositions have been developed. Different binary inorganic salt systems were evaluated according to their properties and their binary phase equilibrium diagram characteristics. Among them, NaNO3-NaOH and KNO3-NaNO3 were identified as the best candidates for thermal storage, according to their high effectivity index and low cryoscopy constant. In addition the rheological behaviors of the solid-liquid mixture were studied to control the viscosity of the slurries during solidification and remelting processes.

11:20 AM

(ENERGY-019-2010) Advanced Composite Materials Enable Effective Energy Capture from Thin Film and High Efficiency Solar Cells

M. Tupper*, P. Keller, R. Taylor, R. Barrett, D. Turse, W. Francis, CTD, United States

New developments in thin film and high efficiency solar cells are improving the capture of solar energy with photovoltaic cells. Large installations of solar arrays are being installed in many locations including at airports, public buildings, schools, and universities as well as at private residences. However a large market that is currently underserved by solar energy is that of remote and mobile power units that can be used in replacement of diesel generators. Based on a Roll out and Passively Deployed Array (RAPDAR), developed for on-orbit deployable satellite solar arrays for satellites, a composite structure and solar cell integration techniques based on the RAPDAR design can be used for terrestrial use. This terrestrial based solar array can be packaged very efficiently. For example, a tennis court sized solar array that can offer over 10 kW a power can be packaged into the size of a large golf bag. A 10 kW diesel generator will weigh over 1500 pounds. Use of solar arrays in remote locations by the military, emergency and disaster response teams, and recreationalist can significantly reduce the green house gases generated by diesel generators as well as to reduce the cost, in both money and lives of delivering diesel fuel to these remote locations.

11:40 AM

(ENERGY-020-2010) Materials Selection and Processing for Lunar-based Space Solar Power

P. J. Schubert*, Packer Engineering, Inc., United States

The ultimate form of solar power is to collect sunlight in space where there is no night, no clouds, and no atmosphere. Low-density radio waves can transmit this power to earth-based receivers, invert the power, and couple it to the grid. This low-pollution power source can be scaled to the entirety of human enterprise. Until recently, economics argued against space solar power (SSP), because launch costs of the megatons of materials are prohibitive. A new approach is to use lunar materials for the bulk of SSP mass. The moon is 21% silicon, which can be formed into solar panels. Several new innovations make possible economical production of electric power from space, provided key materials challenges can be overcome. This paper reviews the ultra-high temperature ceramics and metals required for lunar-based SSP, and some of the laboratory results from experiments to build factories which, when landed on the moon, will produce many times their launch mass in valuable solar panels and array infrastructure.

Hydrogen

High Capacity Materials for Hydrogen Storage

Room: Seashore Ballroom
Session Chairs: Ewa Ronnebro, Pacific Northwest National Laboratory; Ragaiy Zidan, Savannah River National Laboratory

8:00 AM

(ENERGY-021-2010) Development of Processes for the Reversible Dehydrogenation of High Hydrogen Capacity Complex Hydrides (Invited)

G. Severa, University of Hawaii at Manoa, United States; E. Ronnebro, Sandia National Laboratories, United States; X. Liu, G. McGrady, H. Langmi, University of New Brunswick, Canada; C. M. Jensen*, University of Hawaii at Manoa, United States

The majority of current research on the development hydrogen carriers is focused on the quest for new materials. Alternatively, we have found that the development of new chemical processes and/or control of reaction pathways that will enable sustainable hydrogen cycling in well-known high-capacity materials is an equally valid approach. For example, we have recently developed a method for the direct hydrogenation of LiH and Al metal to LiAlH4 that is remarkably convenient and energy efficient. The key to our process was the identification of liquid dimethyl ether as a solvent that is sufficiently coordinating to support the nascent LiAlH4 in the reaction environment, yet volatile enough to be removed easily once it has served this purpose. The discovery of this process opens the door to the application of Ti-doped LiAlH4 as a reversible hydrogen storage material that can reversible release up to 7 wt% hydrogen commencing at temperatures as low as 80 °C and subsequently be recharged almost quantitatively at room temperature and moderate pressures. Our simplification of the hydrogenation half-cycle may provide the key to harnessing the long-recognized potential of this lightweight, high capacity material as a practical hydrogen carrier. We have also, for the first time, demonstrated the hydrogenation of MgB2 to Mg(BH4)2.

8:20 AM

(ENERGY-022-2010) Development of hybrid tank system and investigation of hydrogen absorbing alloys

E. Akiba*, K. Asano, AIST, Japan; T. Fuura, S. Tsunokake, Japan Metals and Chemicals, Japan; Y. Sakaguchi, SAMTECH, Japan; M. Monde, Saga University, Japan

Major on board hydrogen storage methods are compressed gas, liquid hydrogen and hydrogen storage materials. However, at present any of single methods meet the requirements from vehicular application. The hybrid tank system is combination of hydrogen storage materials and compressed gas. Kuriyama et al. have proposed the concept of the system and demonstrations using real size tanks have been carried out by Toyota Motor Co. Development of the tank system has been conducted under the Japanese national project and materials for the hybrid tank are also investigated. In the hybrid tank, hydrogen pressure reaches to 35 MPa in some cases but there is little work in this pressure region so far. In this paper, recent progress in fabrication of the hybrid tank and in material investigation is introduced.

8:40 AM

(ENERGY-023-2010) Factors Affecting Hydrogen Release from Metal Borohydrides

V. Stavila*, Sandia National Laboratories, United States; E. H. Majzoub, University of Missouri, United States; S. Hwang, California Institute of Technology, United States; R. J. Newhouse, University of California Santa Cruz, United States; M. Ulutagay-Kartin, W. Luo, J. G. Cordaro, Sandia National Laboratories, United States; T. J. Udovic, National Institute of Standards and Technology, United States

Practical hydrogen storage for transportation purposes requires materials that exhibit high hydrogen capacity, low decomposition temperatures, and fast kinetics for both hydrogen release and absorption. Unfortunately, to date there is no known material that possesses all of these attributes. Metal borohydrides are considered for hydrogen storage applications due to their high gravimetric and volumetric hydrogen densities, however high dehydrogenation temperatures, slow kinetics and limited reversibility represent serious obstacles in developing practical storage systems based on these materials. Here we present our recent efforts aimed at understanding the factors that affect the stability and thermal decomposition pathways of metal borohydrides. We present examples that illustrate both thermodynamic and kinetic factors which govern the hydrogen release from a range of metal borohydride materials, including LiBH4, Mg(BH4)2, Ca(BH4)2 and Ti(BH4)3.

9:00 AM

(ENERGY-024-2010) Synthesis of alkali amidoborane for hydrogen storage

Z. Xiong*, G. Wu, J. Guo, H. Chu, C. Wu, Dalian Institute of Chemical Physics, China; Y. Chua, National University of Singapore, Singapore; P. Chen, Dalian Institute of Chemical Physics, China

Recent researches on hydrogen storage were extensively given to chemical hydrides comprised of light elements and having high hydrogen content. Holding a hydrogen capacity of 19.6 wt%, ammonia borane (NH3BH3) shows potential to be a hydrogen storage material. Our recent effort in modifying NH3BH3 by replacing one of its H in NH3 group with alkali metal successfully produced lithium amidoborane (LiNH2BH3) and sodium amidoborane (NaNH2BH3). Temperature Programmed Desorption and volumetric release measurements showed amidoboranes evolved 2 equiv. H2 in two steps; a burst was observed around 90 dergreeC and a broad desorption signal centralized at 150 degreeC. Borazine was undetectable. DSC indicated mild exothermic nature of that burst and the second dehydrogenation process was nearly thermal neutral. Therefore, isothermally heating LiNH2BH3 and NaNH2BH3 at 91 degreeC for 19h resulted in the evolution of 10.7wt% and 7.4wt% hydrogen, respectively. More recently, NH3 co-produced in the dehydrogenation of amidoborane was quantitatively measured for practical purpose. It was found that NH3, though produced in a concentration of 1000-2000ppm at the initial heating stage, was quickly consumed in secondary reaction in close system resulting in a decrease of concentration to tens ppm at the completion of dehydrogenation.

9:20 AM

(ENERGY-025-2010) Enhancing the Hydriding and Dehydriding Kinetics of $LiBH_4$+MgH_2 Systems via the Addition of Transition Metals

X. Wan*, K. Crosby, Y. Zhong, L. L. Shaw, University of Connecticut, United States

Currently, $LiBH_4$ has been studied extensively as a reversible hydrogen storage material for mobile applications because of its high gravimetric density. Furthermore, the addition of MgH_2 can thermodynamically destabilize $LiBH_4$. However, the hydriding and dehydriding kinetics of the $LiBH_4$+MgH_2 system are still very slow. In this study, transition metals, including Mn and V, are added to the $LiBH_4$+MgH_2 system via high-energy ball milling to enhance its dehydriding and hydriding properties. It is shown that the addition of V can enhance the dehydriding rate and lead to a larger amount of hydrogen released (3.3 wt%) below the melting point of $LiBH_4$. In contrast, the addition of Mn substantially increases the hydrogen uptake rate at the temperature range between 190 to 250^{o}C. From XRD, FTIR and NMR analyses, we believe that the V additive enhances the decomposition of MgH_2, which in turn promotes the hydrogen release of $LiBH_4$ at a lower temperature. However, the role of the Mn additive is different; it dissolves in the MgB_2 solid solution and increases the diffusion coefficient of the rate-limiting species during the hydriding process.

9:40 AM

(ENERGY-026-2010) Adduct-stabilized aluminum borohydride as advanced hydrogen storage materials

D. A. Knight*, R. Zidan, C. Fewox, T. Motyka, Savannah River National Laboratory, United States; R. Mohtadi, P. Sivasubramanian, Toyota Research Institute of North America, United States

Metal borohydrides show great promise for use as hydrogen storage materials in having the largest hydrogen capacity of all the complex hydrides. Aluminum borohydride, [Al(BH4)3,], possesses one of the highest hydrogen capacities, having almost 17 wt. % hydrogen available for desorption. Nevertheless, the practicality of this material is in question since it is not only a volatile and pyrophoric liquid at room temperature but it also tends to emit large amounts of poisonous diborane during the desorption process. Previous studies have shown that Al(BH4)3 will combine with a variety of Lewis bases to form a more stable and manageable solids. Still, there have been only limited investigations of these adducts abilities as viable materials for productive hydrogen release and absorption. Presented here is the synthesis and hydrogen desorption/absorption analysis of selected Al(BH4)3/Lewis base adducts, along with in-depth characterization in order to obtain a more accurate description of the materials' molecular structure and to determine a plausible desorption mechanism. The materials hydrogen sorption capabilities are measured using a standard Sieverts apparatus with additional thermal characteristics examined by TGA coupled with residual gas analysis. The materials and the associated sorption products are further characterized by X-ray powder diffraction, XRPD, Raman and FT-IR spectroscopy.

10:20 AM

(ENERGY-027-2010) Forming and Regenerating Alane using Electrochemical Cycle (Invited)

R. Zidan*, Savannah River National Laboratory, United States

Aluminium hydride, AlH3, also known as alane has high capacity (10.1 mass% H2) and (149 kg H2/m3) density. In addition, rapid hydrogen release from alane can be achieved using only the waste heat from a fuel cell or a hydrogen internal combustion engine. The direct hydrogenation of aluminum to alane requires over 100,000 bars of hydrogen pressure at room temperature. Alane can be also produced through chemical synthesis that typically produces stable metal halide such as LiCl. The impracticality of using such high pressure or having stable by-products has precluded alane from being used as a reversible hydrogen storage material. We present a cycle based on electrolysis and catalytic hydrogenation to avoid either the impractical high hydrogen pressure needed for hydriding aluminium or the formation of stable by-products, using the chemical rout. A reversible cycle to form alane electrochemically using NaAlH4 in THF has been successfully demonstrated. To complete the cycle, the starting alanate can be regenerated by direct hydrogenation of the dehydrided alane and the alkali hydride (NaH). Alane produced by the electrochemical method was characterized using TGA, XRD and Raman spectroscopy.

10:40 AM

(ENERGY-028-2010) Tuning complex metal hydrides properties for onboard hydrogen storage application (Invited)

R. Mohtadi*, P. Sivasubramanian, Toyota Research Institute of North America, United States; J. Gray, R. Zidan, Savannah River National Laboratory, United States

Currently, hydrogen is being stored on board automobiles either using high pressure compressed hydrogen tanks at 350 or 700 baror by using liquid hydrogen stored at 20 degrees Kelvin. These systems suffer from low hydrogen volumetric storage density, which is the case for the high pressure tanks or hydrogen boil off problems, as is the case for liquid hydrogen, making these systems impractical for onboard storage. On the other hand, storage of chemically bonded hydrogen in materials like complex metal hydrides, such as alanates or borohydrides, considerably enhances the materials hydrogen volumetric density. Currently, global research efforts are focused on improving the hydrogen storage properties in these materials including enhancing their gravimetric density, dehydrogenation thermodynamics, kinetics, and reversibility. However, one key challenge against their utilization is the thermodynamic and kinetic barriers of hydrogen charge and discharge In the work we will present, we will share our research efforts targeting the modification of complex hydrides thermal properties. We will show our concept targeting the formation of intermediate stability complex hydrides by combining a high thermodynamic stability borohydride such as LiBH4 with lower stability alanates. We will show the thermal property enhancement findings we obtained and discuss our progress to date.

11:00 AM

(ENERGY-029-2010) Solid State Chemical Hydrogen Storage in NHxBHx Materials (Invited)

A. Karkamkar, T. Autrey*, Pacific Northwest National Laboratory, United States

The NHxBHx class of compounds may be classified as complex hydrides and/or chemical hydrogen storage materials. Chemical hydrogen storage materials are of great interest for on-board hydrogen storage because they are capable of providing large quantities of hydrogen with rapid kinetics at moderate temperatures. Our group has been working on developing an in-depth understanding of the chemical and physical properties of amine borane materials for solid state on-board hydrogen storage. These materials, (NHxBHx) provide both high gravimetric and volumetric densities of hydrogen. Hydrogen is released at low temperatures through a series of moderate exothermic reactions. In this work we present experimental studies designed to elucidate more details about the potential mechanism for H2 formation from NHxBHx compounds in the solid state and in solution.

11:20 AM

(ENERGY-030-2010) Multicomponent hydrogen storage materials based on LiBH4 (Invited)

G. Walker*, University of Nottingham, United Kingdom

Lithium tetrahydridoborate, LiBH4, is of interest for solid state hydrogen storage because it has a high volumetric and gravimeteric storage capacity, 0.12 kg(H2)L-1 and 18.5 wt.%, respectively. However, temperatures above 500°C are needed to drive off all the hydrogen. In order to reduce the temperature of dehydrogenation, destabilisation agents have been investigated for rapid low temperature evolution of hydrogen. Destabilisation enables the thermodynamics to be tailored to yield lower temperatures at which 1 bar hydrogen can be evolved, T(1bar). Two classes of destabilisation agents have been investigated: metal oxides and metal hydrides. A range of oxides have been studied and the type of oxide and the stoichiometry of the mixture plays a significant role on the dehydrogenation mechanism. The onset temperature of dehydrogenation has been reduced to 150°C. The LiBH4-MgH2 system has also been investigated because this system has a T(1bar) of ca. 170°C. It has been found that the stoichiometry of the mixture has a significant impact on the cycling kinetics with MgH2-rich systems exhibiting much faster kinetics. The effect of hydrogen pressure has been investigated on the reaction pathway which has been found to have a significant effect on the cycling kinetics. The LiBH4-MgH2 system has been extended to investigate the effect of other hydride materials.

11:40 AM

(ENERGY-031-2010) Decomposition behaviour of metal borohydride compounds (Invited)

D. Book*, D. Reed, University of Birmingham, United Kingdom

There is great interest in the potential hydrogen storage properties of borohydrides such as $LiBH_4$, $Ca(BH_4)_2$ and $Mg(BH_4)_2$, both in terms of the compounds on their own, or for their use in reactive hydride composites (e.g. $LiBH_4/MgH_2$). For both approaches, a greater understanding of the nature, kinetics and thermodynamics of the phases formed during decomposition is essential. We have used dispersive Raman spectroscopy with a sample cell that allows in situ measurements in an argon atmosphere up to 600°C. Studies on the decomposition of $LiBH_4$, $LiBH_4/MgH_2$ and $Ca(BH_4)_2$, have shown that it is possible to detect amorphous decomposition products such as $Li_2B_{12}H_{12}$ and CaB_6 in situ (at temperature). In the case of $LiBH_4$, in situ microstructural observations have also been made. These results are shown in the context of in situ XRD, TPD and DSC results, with a view to identifying the various available reaction pathways.

Battery Technology

Energy Storage and Conversion I

Room: Sawgrass
Session Chair: Thad Adams, Savannah River National Lab

8:00 AM

(ENERGY-032-2010) Free Standing Nanostructured Anodes for Li-Ion Batteries (Invited)

M. Au*, T. Adams, Savannah River National Laboratory, United States; Y. Zhao, University of Georgia, United States

Currently, carbon base anodes are being used for Li-ion rechargeable batteries through Li ion intercalation process. The theoretic capacity is limited at 372 mAh/g. Searching for new anode materials that possesses higher energy storage capacity and inherent fire safety is not only scientist's passion, but the mandate of industries and customers, particularly for plug-in hybrid vehicles and portable power sources. It is found that metal oxides and metals can host Li ions through conversion process. The theoretic capacity of metal oxides and metals is in the range of 500 ~ 4000 mAh/g.. The aligned nanostructure, such as nanorods, creates large inter-rods space that is capable to store the charges and accommodates the volume expansion caused by conversion. It is expected the aligned nanorods of metal oxides will offer high energy and power density and inherent safety. Growing free standing nanostructured anode materials on current collectors directly without additives and binders represent a new trend of anode fabrication with simplified process and low cost. The aligned nanostructures were used as the anodes directly without additives and binders. In the cell tests, the nanostructured metals/metal oxides anodes demonstrated 1000 – 1500 mAh/g reversible energy densities at high discharge rates. We will present our experimental results and discuss the aspects related to practical applications in the conference.

8:40 AM

(ENERGY-033-2010) Modeling nanoparticle synthesis by gas condensation in a nanocluster source for applications in photovoltaic and hydrogen fuel cells

E. Pauliac-Vaujour*, E. Quesnel, V. Muffato, CEA Grenoble, France

One challenging and relatively cost-effective alternative to MOCVD-deposited nanoparticles (NPs) is the synthesis of NPs by inert-gas condensation of a sputtered vapor in a dedicated magnetron-based reactor. By tuning the collision path length and hence the time of residence of NPs in the carrier gas phase, spherical nano-aggregates with well-controlled nanometer-scale diameters and relatively narrow size dispersion are produced from various materials. Such aggregates exhibit interesting properties related to their high surface-to-volume ratio and surface reactivity (e.g. in catalysis applications). On the basis of experimental results, a detailed modeling of NP nucleation and growth based on the classical nucleation theory was developed taking the peculiar geometry and thermal profile of the NP reactor into account. The simulated curves, calculated by a matlab© program developed for that purpose, exhibit a good qualitative agreement with experiment and highlight the role of the process parameters and reactor temperature profile on the NP size distribution. Such calculations underline the possible optimization of the NP source design in order to improve its efficiency and reproducibility. The model may also yield a feasibility criterion and facilitate process development for costly materials by reducing the range of investigated parameters.

9:00 AM

(ENERGY-034-2010) Nano-aggregate synthesis by gas condensation in a magnetron source for efficient energy conversion devices

E. Pauliac-Vaujour*, E. Quesnel, V. Muffato, R. Najjar, N. Baclet, R. Bouchmila, P. Fugier, CEA Grenoble, France

The yield of energy-converting devices such as fuel cells – that produce electrical power from chemical energy – is generally enhanced by the presence of a catalyst, whose nature and structure must comply with very strict specifications. A challenge in reducing the fabrication cost of these devices is to increase their active surface area while decreasing the amount of material used as a catalyst (e.g. Pt compounds and alloys for fuel cells). An alternative to MOCVD is a commercial magnetron-based inert-gas-condensation source, which limits material consumption by reducing the catalyst load by a factor of at least 10 while increasing the texturing of the active surface area. 4nm PtCo nanoparticles (NPs) were deposited onto a fuel cell gas diffusion layer with an excellent control on size dispersion. The fabrication process was optimized prior to experiment via a predictive model of the NP nucleation and growth within the dedicated nano-cluster source. No coalescence of the spherical NPs was observed following deposition, so that the fine texturing of the surface was preserved. The amount of deposited material may be accurately varied from far-less than a monolayer up to tens of $\mu g/cm^2$ depending on the applications, for instance surface plasmon enhanced absorption and quantum dots for photovoltaic cells or catalysis for heat dissipation in microelectronics among others.

9:20 AM

(ENERGY-035-2010) Multi-walled Carbon Nanotubes Functionalized by Carboxylic Groups: Activation of TiO2 (Anatase) and Phosphate Olivines (LiMnPO4, LiFePO4) for Electrochemical Li-storage

L. Kavan*, J HEYROVSKY INSTITUTE, Czech Republic

Multi-walled carbon nanotubes functionalized by carboxylic groups, exhibit better affinity towards TiO2 (P90, Degussa) as compared to that of pristine MWNT. Also the electrochemical performance of TiO2 is improved by nanotube networking, but the Li-storage capacity of TiO2 is unchanged. Whereas the composite of TiO2 with non-functionalized nanotubes demonstrates simple superposition of the behavior of pure components, the composite with functionalized nanotubes has unique faradaic pseudocapacitance which is specific for this composite only. The surface functionalization of MWNT enhances charge storage capacity and reversibility of a composite with LiMnPO4 (olivine), but mediates also the electrolyte breakdown at potentials >4.2 V. Whereas the electrochemical activation of LiMnPO4 (olivine) by functionalized MWNT is quite modest, excellent performance was found for LiFePO4 (olivine) in composite materials containing only 2wt% of functionalized nanotubes.

9:40 AM

(ENERGY-036-2010) Nanofibrous TiO2: A new material with extraordinary properties

M. Zukalova*, L. Kavan, J. Prochazka, JHIPCH, Czech Republic

Nanofibrous TiO2 prepared by means of electrospinning represents a novel material with specific properties resulting from its unique morphology. Anatase or rutile nanofibres exhibit "shape memory". Their shape withstands both high temperature annealing (800oC) and even chemical transformation. Hence, the product of the reaction of nanofibrous anatase with ammonia in gas phase is nanofibrous TiNxOy.The conversion of nanofibrous TiO2 to TiNxOy is completed at about 500oC due to its enhanced chemical reactivity. This conversion is fully reversible; the product of the back reaction is again nanofibrous TiO2. Fibrous anatase has been recently used as a component improving the performance of dye sensitized solar cells; fibrous TiNxOy is a material of huge application potential due to its high electric conductivity, and hardness.

10:20 AM

(ENERGY-037-2010) Ferrocene based carbon–Iron/lithium fluoride nanocomposite as stable electrode material in lithium batteries (Invited)

R. Prakash*, M. Fichtner, Karlsruhe Institute of Technology, Germany

An incessant increase of mobile electronic devices requires high-energy density Li-ion batteries. The energy density of a battery intimately depends on the properties of electrode materials. The fundamental way to attain high capacity is to utilize all possible oxidation states of the electrode material by reversible conversion reaction. High capacity was observed in nanocomposites with transition metal oxides using such a conversion reaction that involves their reduction to nanosized metal, and lithium oxides. Although transition metal fluorides have higher theoretical energy densities than oxides, only little efforts have been made due to their poor electronic conductivity. Recently, reversible electrochemical activities of metal fluorides nanocomposites (TiF3, VF3, FeF3, CoF3, BiF3, etc) have been reported. Some of these exhibited reversible specific capacities as high as 600 mAh/g. However, the application of metal fluoride cathodes is still hampered by their reaction irreversibility, poor cycling stability, and in some cases requires high temperature to attain this value. Incorporation of transition metal/fluorides into nanocarbons is considered to be an effective method to improve cycling performance. In this respect, carbon nanotubes, catalytically grown carbon fibers, porous carbon materials, and graphitic carbons have gained much attention. Herein we present our efforts to obtain iron-confined-nanocarbon/LiF nanocomposite from an appropriate mixture of ferrocene and LiF by thermal treatment at 700 °C in a closed reactor under argon atmosphere. The nanocomposite produced consists of multi-walled carbon nanotubes and onion-type graphite structures in which iron particles are encapsulated, and LiF is dispersed throughout the matrix. The nanocomposite employed as the cathode of a Li battery exhibited a reversible capacity of 280 mAh/g in the potential range 0.5-4.3 V and of 170 mAh/g in the range of 1.3-4.3 V at a current density of 20.83 mA/g. The nanocomposite cathode showed capacity retention of 83.5% after 200 cycles, as well as a durable rate capability. However, efforts are in progress to optimize the Fe and carbon contents of the nanocomposite in order to increase the capacity of the system.

11:00 AM

(ENERGY-038-2010) New Channel Structure Materials for Cathodes of Li Batteries: Processing and Structural Investigations

C. Kallfass, Max Planck Gesellschaft, Germany; S. Hermann, Technische Universität Berlin, Germany, Technische Universität Berlin, GermanyMax Planck Gesellschaft, Germany; H. Schubert*, Technische Universität Berlin, Germany

The electrodes for Li batteries are mostly based either on olivine or spinell structures. They are prone to a first order phase transformation on loading by Li ions, which results strain and stresses. The electrodes are loosing structural integrity and function. This paper, however, reports the experience of a new channel type electrode material based on a Li-Fe/Mn phosphate Arrojadite. The structure contains stable channels. Thus, only a small structural reaction on the Li penetration was observed. NMR showed Li as a part of the structure. TEM EELS showed a reaction of the Fe/Mn site but a direct measurement on the changes of Li charge during penetration failed. A neutron structure determination of a Li loaded structrue is in progress. A demonstrator cell has been built up. The most positive property was a very high number of achievable loading cycles reaching up to 10000, compared to 750 for conventional materials. The cell showed about 3.7 V loading voltage for the Fe and 4.3 V for the Mn system. The battery does not contain toxic components.

11:20 AM

(ENERGY-039-2010) Graphite coated with SiCN ceramic: can one explain the enhanced electrochemical properties of this anode material by understanding the lithium diffusion mechanism?

A. P. Nowak*, M. Graczyk-Zajac, C. Fasel, R. Riedel, Darmstadt University of Technology, Germany

Commercially used anode materials for lithium-ion batteries are based on graphite and ensure stable, reversible capacity of ~360 mAh/g. However, for high charge/discharge (>1C) rates this capacity is fading. We have found that the capacity of graphite coated with SiCN based ceramic is much higher than pure graphite and can reach 600 mAh/g. We have demonstrated that composite electrode can be discharged with more than 2 C rate, without noticeable capacity losses. High discharge capability is less influenced by electrode loading. A correlation between the electrode capacity, its high rate capability, the starting ratio graphite/polymer, the pyrolysis temperature and material composition has been established. In order to better understand this phenomenon we have calculated the diffusion coefficient of lithium in pure graphite and in our graphite/SiCN composite materials. The diffusion coefficient as function of the electrode potential was calculated on the basis of electrochemical impedance spectroscopy, cyclic voltammetry and galvanostatic intermittent titration technique. Diffusion coefficients have been measured for our SiCN containing composites synthesized at various temperatures. Direct dependence between the lithium diffusion and the materials electrochemical properties has been elaborated.

11:40 AM

(ENERGY-040-2010) TiO2 Brookite as anode for lithium ion batteries

D. Dambournet*, I. Belharouak, K. Amine, Argonne National Laboratory, United States

Lithium-ion batteries are now facing the challenge of meeting the energy and power requirements for plug-in hybrid vehicles and electric vehicles. With regard to the negative electrode, titanium oxide (titania) is an interesting alternative anode to graphite due to its operating voltage (~1.5 V), which may enable extended cycle life as well as enhanced safety. TiO2 displays different structural arrangements including the well-known anatase and rutile forms. Only few articles are related to the use of the Brookite as anode in lithium ion batteries. This is due to the difficulty to prepare such a phase. This work will present a new and simple method to prepare the metastable TiO2 Brookite which consists of (i) an aqueous precipitation of the titanium oxalate Ti2O3(H2O)2(C2O4).H2O and (ii) the isolation of TiO2 Brookite by thermal decomposition of the titanium oxalate. The morphology of the prepared brookite is very original with TiO2 nanodomains embedded in large micron-size mesoporous particles and exhibiting a high specific surface area of 255 m2/g. This original morphology enables a good dispersibility suitable during the fabrication of the electrode and a unique combination of a high specific surface area and a high packing density leading to high gravimetric and volumetric capacities. The talk will describe the synthesis and characterizations of the precursor as well as the electrochemical properties of the TiO2 brookite.

Nuclear

Nuclear Fuels

Room: Dunes 1&2
Session Chairs: Robert Sindelar, Savannah River National Laboratory; Kenneth McClellan, Los Alamos National Lab

8:00 AM

(ENERGY-041-2010) Overview of Materials Challenges for Nuclear Fuels (Invited)

K. J. McClellan*, Los Alamos National Lab, United States

Nuclear fuels are prime examples of materials in extreme conditions, but these materials must also perform in an acceptable and predictable manner. Typical fuel pins are multi-component systems consisting of the fuel itself containing the fissile species, a heat transfer medium, and cladding to contain the fuel, fission products and fission gasses created during service. Each of the components and the overall system is subject to complex and evolving chemistry and thermal conditions while experiencing substantial radiation damage. This talk will provide context for the Nuclear Fuels session with an overview of materials challenges for thermal and fast spectrum reactors with examples from specific, relevant fuels systems.

8:20 AM

(ENERGY-042-2010) Advanced Carbide and Nitride Nuclear Fuels (Invited)

J. Carmack*, S. L. Hayes, Idaho National Laboratory, United States

Ceramic nuclear fuels are used almost exclusively in currently operating nuclear power plants throughout the world. Although metallic fuels have been developed to high confidence levels, primarily for fast reactor applications, advancements to the oxide fuel system continue to be the focus of many research and development programs. The carbide and nitride fuel systems have been studied since the 1960s, primarily for use in liquid metal cooled fast breeder reactor (LMFBR) applications. Initial interest was motivated by the high metal atom density of both the carbide and nitride fuels relative to oxide fuel, which makes possible a substantially higher breeding ratio and lower doubling time. Interest in these fuels was sustained well into the 1980s due to their potentially superior combination of thermo-physical properties relative to both metal and oxide fuels: namely, high fissile density, high thermal conductivity, and high melting point. Additionally, both carbide and nitride fuels can be fabricated with either a small, helium-bonded fuel/cladding gap or a large, sodium-bonded gap. In many respects, they embody some of the best attributes of both metal and oxide fuel systems. The purpose of this paper is to provide an overview of the performance attributes of carbide and nitride fuels and to provide a summary of the irradiation experience and knowledge base that exists. The primary performance behavior of each fuel system will be discussed. The development challenges remaining that will determine the future success of these fuel systems will then be reviewed and discussed. This manuscript has been authored by a contractor of the U.S. Government for the U.S. Department of Energy, Office of Nuclear Energy, Science, and Technology (NE), under DOE-NE Idaho Operations Office Contract DE AC07 05ID14517. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

8:40 AM

(ENERGY-043-2010) Material Challenges for Particle Nuclear Fuel Technology

S. Voit*, G. DelCul, R. Hunt, Oak Ridge National Laboratory, United States

The present nuclear energy fuel economy is based on a uranium oxide fuel form; Light Water Reactor (LWR) UO2, Heavy Water Reactor (HWR) UO2, and Mixed Oxide (MOX) UPuO2. There is significant knowledgebase and performance history with uranium oxide fuels operating in present day Generation II and III reactors; however, there is a need to develop advanced fuels and transmutation targets to support Generation IV reactors and a closed fuel cycle. These advanced fuels will need to operate to higher burn up and in more extreme environments thus they will present a host of materials challenges and require a better understanding of fuel materials thermophysical and thermochemical behavior. Particle fuel technologies are being considered for the development of candidate advanced fuel and target forms. Particle fuel/target forms include coated particles such as the tristructural-isotropic (TRISO) and uncoated particles such as sphere-pac. Material challenges associated with particle fuels include fabrication challenges, understanding mechanisms for phase formation and stability, microstructural evolution, and Fuel Clad Chemical Interaction (FCCI) and Fuel Clad Mechanical Interaction (FCMI). This paper will present a historical overview of particle fuel technologies and highlight some of the material challenges that must be overcome before these technologies can be used to support a nuclear renaissance.

9:00 AM

(ENERGY-044-2010) Metal Fuel Development within the Fuel Cycle Research and Development Program (Invited)

J. Kennedy*, T. O'Holleran, J. I. Cole, D. E. Janney, R. Fielding, R. Mariani, C. Papesch, M. K. Fig, Idaho National Laboratory, United States

Metal alloy fuels are under consideration for the transmutation of minor actinides in fast spectrum reactors within the framework of the Fuel Cycle Research and Development (FCRD) program in the USA. Although very good fuel performance has been long demonstrated for U-Zr and U-Pu-Zr fuels, the increased compositional complexity of the U-Pu-Np-Am-Zr transmutation fuels offer additional materials challenges. The deficit level of documentation and fundamental understanding of the properties of the actinides and actinide systems is a lead challenge for these materials. Following this is the issue of material interactions. Although over 130,000 fuel pins were successfully cast for the EBR-II reactor (including ~30,000 slugs case under remote hot cell recycle conditions), the silica molds employed created a significant waste stream. Since one of the requirements for the transmutation fuels is to minimize waste generation, reusable molds and crucibles are needed, yet the aggressive nature of molten zirconium and actinides towards many typical mold/crucible materials is a challenge. Besides stabilizing an isotropic type structure, the Zr plays a crucial role in raising the melting point of the fuel. The ubiquitous observation of Zr rich inclusions in the fabricated fuel effectively removes Zr from the fuel phase and lowers the melting temperature. The challenge is to understand the formation of these phases and hinder them in the fabrication. The burn-up requirements of the fuel are related to the initial fissile density, which is related to the Zr content of the fuel. Understanding the influence of the Zr content on the fuel phase(s) formation and corresponding microstructure is a formidable task. For example, at low Zr content (down to 10 wt%) an ζ-phase may predominate whereas at higher Zr content (up to 40 wt%) a δ-phase may predominate. Understanding and controlling the microstructural features of these two phases is important to the fuel performance. Related to this is the very significant fuel material challenge of understanding and possibly controlling the element migration and microstructure evolution of the fuel in reactor, which would depend on the initial composition and microstructure of the fuel. A prime example here is the effect of lanthanide fission product buildup and reprocessing carryover in the metal alloy fuel. Lanthanide precipitates are known to migrate to the fuel-cladding interface and possibly increase the fuel-cladding chemical interaction. In addition, Am will more closely associate with the lanthanide precipitates, thus removing it from the fuel phase(s). Experimental results obtained through the metal alloy development program on these issues will be presented and discussed.

9:20 AM

(ENERGY-045-2010) Materials Issues in Cladding and Duct Reactor Materials

S. Maloy, LANL, United States; M. Toloczko*, PNNL, United States; J. Cole, INL, United States; T. Byun, ORNL, United States

The Fuel Cycle Research and Development program is investigating methods of burning minor actinides in a transmutation fuel. To achieve this goal, the fast reactor core materials (cladding and duct) must be able to withstand very high doses (>300 dpa design goal) while in contact with the coolant and the fuel. Thus, these materials must withstand radiation effects that promote low temperature embrittlement, high temperature helium embrittlement, swelling, accelerated creep, corrosion with the coolant, and chemical interaction with the fuel (FCCI). Research is underway that includes determining radiation effects in ferritic/martensitic steels at doses up to 200 dpa, minimizing FCCI, and developing advanced alloys with improved irradiation resistance. To develop and qualify materials to a total fluence greater than 200 dpa requires development of advanced alloys and irradiations in fast reactors to test these alloys. Test specimens of ferritic/martensitic alloys (T91/HT-9) previously irradiated in the FFTF reactor up to 210 dpa at a temperature range of 350-700°C are presently being tested. This includes analysis of a duct made of HT-9 after irradiation to a total dose of 155 dpa at temperatures from 370 to 510°C. Compact tension, charpy and tensile specimens have been machined from this duct and mechanical testing as well as SANS and Mossbauer spectroscopy are currently being performed.

9:40 AM

(ENERGY-046-2010) Chemical and Phase Behavior of Oxide Fuels for LWR and Fast Nuclear Reactors (Invited)

T. M. Besmann*, S. L. Voit, Oak Ridge National Laboratory, United States

Current interest in higher burn-up/longer-lived fuel for light water reactors and high burn-up fast reactor fuels will necessitate significant efforts to understand fuel behavior and potentially develop new fuel systems. For the envisioned higher burn-ups it means that properties will be much more complex to represent. Behavior within a likely oxide fuel pin is difficult to model owing to the high temperatures, large number of elements and their significant concentrations that are a result of fuels taken to high burn-up. This unprecedented complexity offers an enormous challenge in the thermochemical understanding of these systems and opportunities to advance modeling to describe these materials. This paper will review the behavior of high burnup reactor fuels and what will be needed to understand their performance. This research was sponsored by the U.S. Department of Energy through the Office of Nuclear Energy–Fuel Cycle R&D Program at Oak Ridge National Laboratory under contract DE-AC05-00OR22725 with UT Battelle, LLC.

10:20 AM

(ENERGY-047-2010) How Modeling and Simulation Helps Address Nuclear Fuels Challenges (Invited)

R. W. Grimes*, D. Parfitt, C. Bishop, Imperial College London, United Kingdom

This presentation will focus on the various roles that atomic scale computer simulation can play in developing our understanding of fuel. Throughout it is necessary to bear in mind that modelling of fuels on this scale is immensely challenging; certainly because actinide species are themselves complex to model (the f-electron problem) but also, of course, because simulations must predict something useful about a complex property, which will stem from some diversity of physical and chemical processes. The relationship with experiment is therefore crucial. In fact, simulations will generally address one of three issues. At the most simple level, simulations can be used to fill in gaps between known experimental data, thereby reducing the experimental burden. Second, simulation can be used to predict the role or assess the importance of a known physical process to a fuel process – experimental effort can then be better focused, again reducing the number of experiments. Finally, simulation can be used as a means of rapidly discovering the likely key physical process underpinning a property or change in fuel property. In this case simulation can focus and might actually lead experimental effort: simulation will, of course, not replace experiment but it might become indispensible.

10:40 AM

(ENERGY-048-2010) Microstructure Property Relations in Uranium Oxide

E. Luther*, D. Byler, K. McClellan, P. Papin, H. Volz, K. Lao, Los Alamos National Laboratory, United States

It is well known that ceramic powder feedstocks may vary significantly from source to source and even batch to batch. In order to close the fuel cycle, spent fuel reprocessing will be used to produce powder feedstock that may have unknown and perhaps uncontrolled properties. Strategies for conditioning this feedstock must be developed to keep fabrication processes in control. In this talk, I will describe characterization of nuclear feedstock, powder conditioning methods, consolidation and sintering. Relationships between powder feedstock properties, the processing path and the resulting microstructure will be discussed. LA-UR-09-0652

11:00 AM

(ENERGY-049-2010) Development of Capabilities for Thermal Analysis of Multilayer Materials for Advanced Nuclear Systems

A. T. Nelson*, Los Alamos National Laboratory, United States

Thermal performance of materials within nuclear systems plays a key role in governing the operational parameters of current plants and will establish the thermodynamic efficiencies of next generation designs. Accurate knowledge of baseline thermophysical properties of individual materials is important, but the behavior of multilayer systems is of direct relevance to many design and engineering challenges. Specialized joining methods, fuel-cladding interaction, and advanced thermal or chemical barrier coatings will all act in concert to affect the temperature distribution within a reactor. Specific composite systems that pose challenges within the field of nuclear materials will be profiled with particular attention given to those which remain incompletely understood. The results of ongoing efforts to understand thermal transport across interfaces relevant to the design of nuclear systems as a function of material parameters, temperature, and irradiation will be outlined to convey both current capabilities and limitations. Discussion will conclude with a summary of the near term needs for thermal characterization of multilayer systems necessary for both impending utility power uprates as well as longer term objectives directed toward fuel reprocessing and fusion devices.

11:20 AM

(ENERGY-050-2010) Effect of oxygen stoichiometry on the properties of uranium oxide fuels

D. D. Byler*, K. J. McClellan, E. P. Luther, P. A. Papin, H. M. Volz, Los Alamos National Laboratory, United States; J. B. Henderson, Netzsch Instruments North America, United States

The effects of atmosphere, temperature and stoichiometry of materials have long been of interest to ceramists during sintering because of the many changes that can occur in microstructure and sinterability of the ceramic as a result of small variations. In addition, the attempt to reduce sintering temperature and time for ceramics has been the goal of many researchers to provide an economical means to obtain a high-density product with minimal flaws. This is true for nuclear fuel materials as well. It has been shown that the effects of stoichiometry can contribute to variations up to 750°C in melt point, can allow fuel cladding chemical interaction (FCCI) by oxygen migration to the pellet-cladding interface, and can change the sinterability of the UO2. These variations in the oxygen-to-metal (O/M) ratio need to be controlled to reduce sintering temperatures and provide a means to control the properties of the fuels in service. In this presentation, the effects of O/M on sintering temperatures of UO2 and on properties will be discussed as well as the process being developed to control O/M of the material during sintering.

11:40 AM

(ENERGY-051-2010) The Role of Titanium in Oxide Dispersion Strengthened Alloys for First Wall Structural Materials

G. Sundararajan*, R. Vijay, A. Venugopal Reddy, ARCI, India

Reduced Activation Ferritic/Martensitic(RAFM)steels, Vanadium alloys and SiC composites are under consideration as potential first wall structural materials for the fusion reactors. The technology for manufacture of RAFM steels are well developed. However, RAFM steels undergo significant irradiation related hardening and embrittlement and also exhibit inadequate creep and swelling resistance beyond 800K. In this context,dispersion of nano oxide precipitates in the RAFM steel matrix has proved effective in enhancing the creep and swelling resistance and also the high temperature strength of RAFM steels. Oxide Dispersion Strengthened (ODS) RAFM steels are characterised by nanodispersion of Ti-Y-O clusters/precipitates in a ferritic or martensitic matrix and typically consit of Cr, W, Ti and Yttria as alloying additions.The role of Ti in the ODS-RAFM steel has not been adequately understood though it is generally accepted that it facilitates dispersion of a high number density of nanosized Ti-Y-O precipitates. To further elucidate the role of Ti without the complications arising out of the presence of other alloying elements,two alloys namely, Fe-Yttria and Fe-Ti-Yttria have been prepared by mechanical milling followed by canning and hot extrusion.The microstructural features of these two alloys along with their room and elevated temperature mechanical properties have been evaluated.

Solar

Dye Sensitized Solar Cells and Copper Indium Gallium Selenide based Photovoltaics

Room: Sea Oats
Session Chair: Laura Marshall, ASM International

1:40 PM

(ENERGY-052-2010) Electrical Transport Properties of Lithographically Fabricated Single Titania Nanotube Devices

M. AbdElmoula*, L. Menon, Northeastern University, United States

Electrochemically fabricated titania nanotube arrays are expected to have important applications in solar energy harvesting: high aspect ratio of nanotubes, cheap and scalable fabrication technique, durability and low recombination probability of the electron-hole pairs makes titania nanotubes highly attractive materials for efficient light conversion to electricity. To our knowledge there is no previous report in literature which explores the transport properties of a single titania nanotube to understand the factors that might enhance its transport properties. In this work we have fabricated devices based on released single titania nanotubes. Conducting electrodes have been attached to either end of the nanotubes using e-beam lithography. For such single nanotube devices, we report electrical transport results, first for a blank titania nanotube, where we investigate the effect of wall thickness, tube diameter, tube length and different fabrication routes on the transport properties; second, for gold nanoparticle modified titania nanotubes, where we investigate the effect of coating the nanotubes with gold nanoparticles on the transport properties. This work will provide a clear understanding of charge transport properties in titania nanotubes and how to optimize it for more efficient solar cell fabrication.

2:00 PM

(ENERGY-053-2010) Composite of Nanoanatase Templated Structure and TiO2 Electrospun Nanofibers Improves Parameters of the DSC Anode

J. Prochazka*, L. Kavan, M. Zukalova, JHI, Czech Republic; M. Graetzel, EPFL, Switzerland

High surface area, good anatase crystallinity and high electron conductivity are the essentials needed for a good DSC performance. They are hard to achieve using the TiO2 anode with only one nano-anatase morphology. Synthesis and performance of a composite consisting of electrospun nano-anatase fibers in combination with a P123 templated nano-anatase structure will be demonstrated.

2:20 PM

(ENERGY-054-2010) Hybrid organic flexible solar collectors for smart building construction

J. Iroh*, B. Buschle, J. Logun, E. Obonyo, University of Cincinnati, United States

Flexible solar collectors based on carbon nanofiber reinforced polyaniline are being developed for use in detachable solar cells. The range of the solar spectrum for which the novel organic solar collectors will operate are significantly extended by copolymerization and in-situ reinforcement with appropriate inorganic fillers. One novel feature of the new organic solar collectors is their ease of processability in aqueous or mild organic solvents. Both electrochemical polymerization and chemical oxidative polymerization methods can be used interchangeably to synthesize the hybrid organic solar collectors. Our preliminary results show that the UV-Visible absorbance of the composite organic solar collector encompasses the wavelength range of 290 nm to 800 nm.

2:40 PM

(ENERGY-055-2010) Electrochemical Deposition of CoSb3 Thin Films on Nanostructured Substrate

D. V. Quach*, UC Davis, United States; R. Vidu, AMEROM LLC, United States; J. R. Groza, P. Stroeve, UC Davis, United States

Thermoelectric materials are clean energy conversion materials that show higher figures of merit when the dimensionality is reduced from bulk to ultra thin films and nanowires. Electrochemical deposition is an inexpensive method that has great potential in producing such low-dimension structures. Bulk, partially or fully filled CoSb3 and other skutterudites have shown promising thermoelectric properties but little research has been done on the electrochemical deposition of CoSb3 on nanostructures. Here we report on the electrochemical behavior of CoSb3 skutterudites on nanostructured Au film. Composition and growth mechanism of CoSb3 ultra thin films on nanostructured substrates are discussed in relation to the substrate structures and deposition conditions.

3:00 PM

(ENERGY-056-2010) Suitability of Pyrolytic Boron Nitride, Hot Pressed Boron Nitride, and Pyrolytic Graphite for CIGS Processes

J. Mariner*, W. Fan, X. Liu, C. Raman, J. Leist, Momentive Performance Materials, United States

Pyrolytic boron nitride (PBN), hot pressed boron nitride (hpBN), and pyrolytic graphite (PG) have been studied for chemical and thermal stability in CIGS processing environments. Evaluations are made from Gibb's free energy calculations for BN and C relative to Cu, In, Ga, and Se. Vapor pressure data of BN and graphite is presented and compared with the environments common to both thermal evaporation and to sputtering, as used in CIGS thin film production. The manufacturing processes are explained, that contribute to the stable performance of these materials. The conclusion is supported, that boron nitride and pyrolytic graphite are suitable materials for CIGS processing. Proposals are made of suitable product forms for evaporation sources, heaters, and metal vapor distribution plenums.

3:40 PM

(ENERGY-057-2010) Effect of Elemental Composition on Diffusion of Sulfur into $CuIn_xGa_{1-x}Se_2$ Thin Films

S. A. Pethe*, E. Takahashi, N. G. Dhere, Florida Solar Energy Center, University of Central Florida, United States

In this work the CuInGaSe2 (CIGSe) thin film absorber are prepared by two stage process; first step involves metallic precursor deposition and second step is annealing of the metallic precursors in presence of selenium. For CIGSe thin film solar cell prepared by two stage process, addition of gallium does not result in increase in the open circuit voltage as there is no increase in the bandgap at the surface of the film as it tends to segregate to the back. Sulfurization of CIGSe absorber layer is a bandgap engineering technique. Sulfurization of CIGSe helps to increase the bandgap of the absorber at the interface by shifting the valence band maxima to lower energies. However, excessive sulfur in the bulk of the film may lead to reduction in current, an increase in the series resistance. Hence it is necessary to optimize the sulfurization process to avoid excessive diffusion of sulfur. The purpose of this work was a systematic investigation of sulfur distribution in CIGSe absorbers. Experiments are carried out by varying the stochiometric composition of the absorber film before sulfurization. The variation in Cu/(In+Ga) ratio alters the morphology and structure of the film as well as the sulfur diffusion profile. Efforts are made to correlate the effect of variation in composition and morphology of the film with sulfur diffusion profile in terms of grain boundary and bulk diffusion.

4:00 PM

(ENERGY-058-2010) III-V photovoltaics on flexible metal substrates using biaxially-textured Germanium films

V. Selvamanickam*, A. Freundlich, A. Sundaram, S. Lee, University of Houston, United States; S. Sambandam, A. Rar, X. Xiong, SuperPower, United States

III-V photovoltaics have exhibited efficiencies above 40%, but have found only a limited use because of the high cost of single crystal substrates. At the other end of the spectrum, polycrystalline and amorphous thin film solar cells offer the advantage of low-cost fabrication, but have not yielded high efficiencies. Our program is based on single-crystalline-like thin film photovoltaics on polycrystalline substrates using biaxially-textured templates made by Ion Beam-Assisted Deposition (IBAD). MgO templates made by IBAD on flexible metal substrate have been successfully used for epitaxial growth of germanium films. In spite of a 4.5% lattice mismatch, heteroepitaxial growth of Ge was achieved on CeO2 that was grown on IBAD MgO template. Room temperature optical bandgap of the Ge films was identified at 0.67 eV indicating minimal residual strain. Refraction index and extinction coefficient values were found to match well with that measured from a reference Ge single crystal. GaAs has been successfully grown epitaxially on Ge on metal substrate by molecular beam epitaxy. RHEED patterns indicate self annihilation of antiphase boundaries and the growth of a single domain GaAs. The GaAs is found to exhibit strong photoluminescence signal and, an existence of a relatively narrow (FWHM~20 meV) band-edge excitons measured in this film indicates a good optoelectronic quality of deposited GaAs.

4:20 PM

(ENERGY-059-2010) 200 MeV Ag+ ion beam induced modifications in AgInSe2 films deposited by hot wall vacuum evaporation method

D. Pathak*, R. K. Bedi, Guru Nanak Dev University, India; D. Kaur, Indian Institute of Technology, India; R. Kumar, Inter University Accelerator Centre, India

Hot wall technique was used to prepare AgInSe2 films which work close to thermodynamic equilibrium and therefore considered as most suitable for growth at low temperatures. The samples were grown onto the glass substrate kept at 135°C. The technique can be described as semi closed growth reactor consisting of a vertically mounted quartz cylinder heated by three separately temperature controlled ovens and is closed on the top by the substrate. The first oven heats the source material and control the growth rate, while the second oven heats the wall between source and substrate and the substrate temperature is controlled by the third one. The structural and optical properties of 200 MeV Ag+ ion beam irradiated AgInSe2 films grown by hot wall technique were studied. For pristine samples the band gap was found to be 1.19 and 2.09 eV which is due to the fundamental absorption edge and transition originating from crystal field splitting respectively. Band gap values corresponding to fundamental absorption edge and originating from crystal field splitting show a sharp decrease in values to 1.124 and 1.74 eV respectively, which are explained due to irradiation induced defects.

4:40 PM

(ENERGY-060-2010) Chemical Solution Deposition of IR-Active Thin Films: Epitaxial Growth and Carrier Multiplication

Y. Golan*, Ben Gurion University, Israel

Chemical solution deposition (CSD) is an attractive, inexpensive and industrially scalable technique for depositing thin films that are active in the mid- and near- infrared range. Our studies have shown that thin films of lead selenide and lead sulfide can be deposited with a wide range of microstructures, from nanocrystalline (near IR range) to monocrystalline (mid IR range), the latter with well-defined orientation relations with the underlying substrates (single crystal GaAs and Si wafers). We have recently demonstrated that both our PbS and our PbSe CSD films clearly exhibit carrier multiplication (CM) which is of importance for solar energy conversion. While CM has been thought to be enhanced significantly in nanocrystalline materials such as quantum dots, owing to their discrete energy levels and enhanced Coulomb interactions, we show that contrary to this expectation, for a given photon energy, CM rather occurs more efficiently in our monocrystalline PbS and PbSe films than in nanocrystalline films of the same materials.

Hydrogen

Processing and Applications for Hydrogen Storage

Room: Seashore Ballroom
Session Chairs: Theodore Motyka, Savannah River National Laboratory; Richard Sisson, Worcester Polytechnic Institute

1:40 PM

(ENERGY-061-2010) Large-scale Hydrogen Production by Nuclear Thermochemical Water-splitting (Invited)

W. A. Summers*, Savannah River National Laboratory, United States

A hydrogen economy will require massive amounts of hydrogen. Nuclear energy can be used to split water as a major source of the future hydrogen supply without creation of greenhouse gas emissions. Thermochemical water-splitting, which uses a series of linked chemical reactions that produce hydrogen and oxygen while recycling all intermediate chemicals, has been under development since the early 1970's. Advanced nuclear reactors, such as helium-coooled gas reactors, can provide electricity and heat at temperatures up to 950C to power thermochemical systems. This paper will discuss the development of the Hybrid Sulfur Process, one of the most developed thermochemical cycles. A key component of the process is a sulfur dioxide electrolyzer, which uses PEM fuel cell technology to electrolyzer water while requiring only one-third the electricity of conventional electrolyzers. The products are hydrogen and sulfuric acid, which is in turn thermally decomosed with high temperature heat from a nuclear reactor. Significant progress has been made on the development of both the electrolyzer and the acid thermal decomposition system. Integrated demonstration and process scale-up are being pursued.

2:00 PM

(ENERGY-062-2010) Hydrogen Storage in Glass Capillary Arrays

D. Eliezer*, C.En Ltd., Switzerland

The purpose of the study relates to the development of a viable hydrogen storage technology. Intrinsic to the fulfillment of the potential inherent in hydrogen is the overcoming of obstacles generated by the storage of hydrogen. Conventional storage methods pose volume, weight, safety and monetary obstacles and are unable to meet onboard application goals as defined by the US Department of Energy (DOE). C.En presents an innovative method for the safe storage of highly pressurized hydrogen. It utilizes capillaries made of glass materials, which are cheaper than carbon fibers. Storage tests conducted at BAM, the German Federal Institute for Materials Research and Testing, demonstrated that the technology has a gravimetric storage capacity of 33% and a volumetric capacity of 28 g/L. These results easily surpass the DOE 2015 gravimetric storage targets of 9%. Tests on Borosilicate capillaries were found to withstand 1240 bar pressures, which create a volumetric capacity of 45 g/L, reaching the DOE's 2010 volumetric storage targets. Results indicate a potential resolution to the obstacles inherent in hydrogen storage. The presentation will further delineate upon the theorization and determination of pressure resistance capacities of various glass capillaries, as well as discuss experimental issues regarding the charging, permeation and release of the hydrogen, and the process of refilling capillaries with compressed hydrogen.

2:20 PM

(ENERGY-063-2010) Stress Quenching of Hydrogen in AISI 403 Steel

G. P. Tiwari*, V. D. Alur, Bhabha Atomic Research Centre, India

The present paper describes a technique for electrolytic charging of hydrogen under the influence of tensile stress. The presence of stress affects the ingress and retention of hydrogen within the matrix in two ways. Firstly, it increases several fold the diffusion rates of hydrogen within the matrix. As a result, 10-15 centimeters long steel specimens can be successfully charged with hydrogen within a span of 2-3 days. Secondly, the propensity of hydrogen traps to absorb hydrogen is enhanced considerably. As a result, the net amount of hydrogen retained at the traps is higher than that retained in the absence of stress by 1-2 orders of magnitudes. The most significant aspect of present observation is that a major part of the excess hydrogen trapped under the influence of the stress is retained even after removal of the stress. This phenomenon has been termed as Stress Quenching. To author's knowledge, this is the first reported observation of this kind. Stress quenching can be used to increase the absorption capacity of hydrogen storage materials.

2:40 PM

(ENERGY-064-2010) Production of hydrogen and carbon monoxide from water and carbon dioxide through metal oxide thermochemical cycles

E. N. Coker*, M. Rodriguez, A. Ambrosini, T. Garino, J. E. Miller, Sandia National Laboratories, United States

This work aims to identify the metal oxide phases present during thermochemical cycling and how they change as a function of temperature and gas composition, to aid the design of highly efficient materials for H_2 and CO production. High-temperature X-ray diffraction (HT-XRD) was used to monitor the structure of iron oxides supported on YSZ (10 wt.-% Fe_2O_3 basis) during thermochemical cycling. HT-XRD showed dynamic behavior as iron migrated into and out of YSZ at elevated temperatures, monitored by the lattice parameter of the YSZ. Iron oxides were seen to thermally reduce stepwise from Fe_2O_3 to Fe_3O_4 and finally FeO as the temperature increased from ambient to 1400 °C under He with a low background of O_2. Between 800 and 1100 °C no iron species were detected, indicating that all iron was in solid solution with YSZ. Similar cycles were performed with a cobalt-substituted ferrite which exhibited similar phase evolution. Exposure of $Fe_xCo_{1-x}O$ to CO_2 or air resulted in re-oxidation to $Fe_{3x}Co_{3-3x}O_4$. Thermogravimetric analysis corroborated the reduction/oxidation behavior of the materials during thermal reduction and subsequent reoxidation by H_2O or CO_2. A complimentary study on diffusion of iron oxide into YSZ revealed a steep increase in diffusion rate once temperatures exceeded 1475 °C. Fusion and vaporization of iron species at these high temperatures occurs.

3:00 PM

(ENERGY-065-2010) Concentric Electrode-type On-planar Single-chamber Solid Oxide Fuel Cells

D. Lee*, Yonsei University, Korea, Republic of; H. Kim, Yonsei University, Korea, Republic of; J. Kim, KIST, Korea, Republic of; J. Moon, Yonsei University, Korea, Republic of

Single-chamber solid oxide fuel cells(SC-SOFCs) operate with a mixture of air and fuel. They have shown the alternative way to simplify SOFC systems but also relatively low performances, and their operation mechanisms are not understood in detail. Here, we introduced the novel concentric electrode-type on-planar SC-SOFCs via the micro-fluidic lithography. We investigated the influence of the electrode design on the cell and optimum operation conditions. The yttria-stabilized zirconia(YSZ) electrolyte pellet was fabricated by uni-axial pressing. Poly(dimethylsiloxane)(PDMS) mold was fabricated by the replication of the master pattern of photolithographically prepared SU-8, and was attached on the pellet. The anode suspension, prepared with NiO and YSZ powders, was poured into the reservoir and sintered. The cathode, La0.8Sr0.2MnO3 and YSZ, was fabricated in the same way. Concentric electrode-type cells and linear electrode-type ones were compared in terms of OCV and IV characteristics and impedance analysis. The concentric electrode-type cell showed the higher OCV(max. 0.90V) than the linear-type(max 0.65V). Consequently lower polarization resistance was observed for the concentric electrode-type cell. We confirmed that the electrode design plays a role in the electrocatalytic reaction in the on-planar SC-SOFCs. And the operation mechanism and effective design to maximize the performance were suggested.

3:40 PM

(ENERGY-066-2010) A zero carbon emission method to produce hydrogen and hydrides (Invited)

S. Saxena*, S. Kumar, V. Drozd, FIU, United States

We have modified the SMR (Steam-methane reformation) and coal-gasification techniques of hydrogen production in such a way that hydrogen (and consequently hydride) can be produced at lower energy costs without carbon emission. The reactions used are: 2 NaOH + C + H2O = Na2CO3 + 2 H2 2 NaOH +CH4 +H2O = Na2CO3 + 4 H2 A critical requirement in making this method industrially useful is the fact that the product soda ash can be sold at a price equal to or more than that of the reactant caustic soda. With this cost balance, hydrogen can be produced very cheaply without any carbon emission, provided none of the carbonate is used in a way that it releases the CO2, permitting only low-temperature uses. Several results on the kinetics of the two reactions will be presented. Another method of producing hydrogen is to use the metal-water reaction in such a way that a hydride is produced directly as follows: 2 Mg + H2O = MgH2 + MgO The hydride may then be used with water to produce hydrogen in a variety of physical environments such as transportation vehicles. An important consideration here is that no fossil fuel is used. The method could be economic if the oxide could be reduced at appropriate costs to metal by modern electrolytic methods such as the solid-oxide-membrane process. We will compare the costs of these methods of hydrogen and hydride production and discuss the issues with their possible use for transportation.

4:00 PM

(ENERGY-067-2010) Hydrogen storage materials properties for prototype system concepts (Invited)

E. Ronnebro*, Pacific Northwest National Laboratory, United States

The need for light-weight, high-capacity hydrogen storage materials for transport applications has shifted our focus to alanates, amides and metal borohydrides. During our efforts on discovery and development we identified candidates for reversible reactions by hydrogenating known decomposition products of hydride materials. Although borohydride materials can store ca 11-19 wt% hydrogen, the operation temperatures are high for automotive applications and rehydrogenation kinetics is slow. We have identified pathways for direct hydrogenation of calcium and magnesium borohydrides from their end-decomposition products, opening the door to potential high-capacity hydrogen storage applications. Moving on with applied oriented projects towards subscale prototype tank solutions we at PNNL are currently focusing on systems modeling and materials operating requirements for efficient system concepts for different materials-based technologies including ammonia borane. We are working on upscale synthesis and measuring material properties to fill in gaps in data needed for systems modeling, including parameters such as thermal conductivity, kinetics, thermodynamics and form factor.

4:20 PM

(ENERGY-068-2010) Mechanical Processing as Experimental Tool in Alternative Energy R&D (Invited)

V. P. Balema*, Sigma-Aldrich Corp., United States

Alternative energy is broadly defined as the energy generated in a way that does not deplete natural resources or harm the environment. It is used as an alternative to fossil fuels and non-renewable energy sources such as coal, oil, natural gas or nuclear energy. A possible way to resolve growing energy and environmental problems is the conversion of solar energy into electricity, which can be immediately used to power a variety of tools,or chemically stored in hydrogen-rich substances such as hydrides - the way in which fossil fuels (carbohydrides) formed in nature. Storing energy in hydrogen-rich materials offers a unique opportunity for its convenient and safe use. Unfortunately, none of the hydrogen storage materials currently on the market satisfy requirements of end users, which explains ongoing interest in hydrogen storage R&D. Mechanical milling and grinding have been known as materials processing techniques for hundreds of years. However, systematic studies into their chemical effects began relatively recently. Nowadays, mechanical processing is indispensable for nano-scale design and modification of various hydrogen-rich molecular and ionic solids. This presentation highlights the applications of mechanical processing in basic and applied energy materials research. It also discusses recent discoveries in the area of mechanically induced transformations of molecular and ionic solids.

4:40 PM

(ENERGY-069-2010) Microcrack Resistant Polymers Enabling Lightweight Composite Hydrogen Storage Vessels

M. Tupper*, K. Mallick, J. Cronin, P. Fabian, Composite Technology Development, Inc., United States

Robust, lightweight, storage vessels are needed for on-board storage of hydrogen. Challenges with currently used composite overwrapped vessels include weight due to the non-load bearing liner, performance reliability resulting from separation of the liner, and costs of extra manufacturing steps to fabricate the liner. Linerless composite vessels, where the composite shell serves both as a permeation barrier and a structure, can provide for the lightest weight vessels for a given set of requirements. Preliminary designs show up to 25% weight savings allowing reduced storage system mass and more internal volume. These tanks are targeted to attain hydrogen mass storage efficiency of 15-18% as compared to 3-4% from lined vessels. Manufacturing cost, operational risks and maintenance costs can be reduced due to inherently simple construction. Engineering methods that define material performance requirements, such as polymer strain requirements in a lamina have been used to guide the development of microcrack resistant polymers. Performance of linerless composite tanks has been demonstrated and qualification is on-going.

Nuclear

Waste Forms

Room: Dunes 1&2
Session Chair: John Marra, Savannah River National Lab

1:40 PM

(ENERGY-070-2010) Towards a Global Nuclear Renaissance: A New Paradigm for Waste Management

J. Marra*, Savannah River National Lab, United States

Energy availability is the engine that drives economic growth. With fuel oil and natural gas prices near record highs, and worldwide energy demands increasing at an alarming rate, there is growing international interest in revitalization of nuclear power. In order to achieve the vision of a revitalized nuclear industry, issues associated with waste generation must be addressed and, indeed, must be a primary consideration in any future planning scenario. As part of the United States Department of Energy Global Nuclear Energy Partnership (GNEP), an Integrated Waste Management Strategy is being developed. This strategy considers waste disposition as a primary consideration for any deployment scenario. This presentation describes the critical role that nuclear waste management plays in the future of the international nuclear program.

2:00 PM

(ENERGY-071-2010) Immobilization of Tc in a Metallic Waste Form

W. L. Ebert*, J. C. Cunnane, J. A. Fortner, Argonne National Lab, United States

A multi-phase iron-based metallic waste form is being developed to immobilize the metallic and Tc-bearing waste streams that will be generated during the reprocessing of used nuclear fuels with either aqueous or electrochemical schemes. A metallic waste form permits the efficient processing and immobilization of metallic waste components and may permit higher waste loadings of components that can be readily reduced to metals than other waste forms. These wastes can be processed with added iron (or steel) at about 1600 °C to incorporate transition metal fission products and other waste components in durable solid solution or intermetallic phases. Work is in progress to (1) formulate an alloy composition to immobilize the anticipated range of waste compositions within a small number of phases, (2) identify processing conditions for producing metallic waste forms with high waste loadings and consistent chemical, physical, and radiological properties, and (3) develop a mechanistically-based corrosion and radionuclide release model for calculating the long-term performance of a metallic waste form under the full range of possible disposal conditions. The experimental and modeling approaches will be presented with available results.

2:20 PM

(ENERGY-072-2010) Fabrication and Characterization of an Alloy Waste Form for Used Nuclear Fuel

M. A. Williamson, R. L. Sindelar*, Savannah River National Laboratory, United States

An alloy waste form with noble and transition metal species expected in waste streams from separations processes for used fuel is envisioned for ultimate repository disposal as part of the U.S. integrated waste management strategy. A single iron-based alloy system is being investigated to provide the waste form with the expected set of species. The fabrication and characterization of the waste loading into constituent phases, and dissolution behavior in repository-relevant environments, are reported. The UREX+ (Uranium Extraction +) aqueous processing baseline strategy for the U.S. program includes several waste streams with species that are candidates for an alloy waste form. The initial acid dissolution of the fuel includes metal species termed UDS (Undissolved Solids) that include primarily Zr, Mo, Tc, Ru, Rh, and Pd species. Soluble Tc is also recovered as a solid separate waste specie from the UREX solution using anion exchange. The TMFP (Transition Metal Fission Products) from the TRUEX (Transuranic Extraction) raffinate waste stream, which originates primarily as oxides, include the same species as the UDS, and additionally include Sn and other minor species. Induction furnace melts (~ 50 gram per batch) were made under vacuum at a process temperature of either 1600 or 1700°C for compositions with non-radioactive surrogates of Zr, Mo, Re (for Tc-99), Ru, Rh, Pd, and Sn. The sample compositions were varied in: i) total added Fe or stainless steel; and ii) additional Zr. All species dissolved into the melt at the process conditions, and the resultant ingots were homogeneous across the melt sample volumes. Each of the surrogate waste metal species was incorporated into one or more of the phases in the alloy. The incorporation of the various metal species into the phases caused significant changes in lattice parameters that were evident in the XRD spectra. Electrochemical testing in aqueous solutions at room temperature and pH levels of 3 and 11 with and without added salts were performed to evaluate the corrosion response of the bulk samples (composite microstructure of the phases) at extreme pH conditions and to provide candidate test methods for standardized release rate behavior of the alloy.

2:40 PM

(ENERGY-073-2010) Characterization of a Metallic Zr-Mo Waste Form for Technetium Immobilization

E. C. Buck*, D. Gelles, J. Vienna, Pacific Northwest National Laboratory, United States

Microanalysis using scanning electron microscopy (SEM) and transmission electron microscopy (TEM) has been used to analyze a ~5 g. ingot with composition 71.3 wt% 316SS-5.3 wt% Zr-13.2 wt% Mo-4.0 wt% Rh-6.2 wt% Re prepared at the Idaho National Laboratory. Four phase fields have been identified, two of which are lamellar eutectics, with a fifth possibly present. A Zr rich phase was found distributed as fine precipitate, ~10 μm in diameter, often coating large cavities. A Mo-Fe-Re-Cr lamellar eutectic phase field appears as blocky regions ~30 μm in diameter, surrounded by a Fe-Mo-Cr lamellar eutectic phase field, and that in turn is surrounded by a Zr-Fe-Rh-Mo-Ni phase field. The eutectic phase separation reactions are different. The Mo-Fe-Re-Cr lamellar eutectic appears a result of austenitic steel forming at lower volume fraction within an Mo-Fe-Re intermetallic phase, whereas the Fe-Mo-Cr lamellar eutectic may be a result of the same intermetallic phase forming within a ferritic steel phase. Cavitation may have arisen either as a result of bubbles, or from loss of equiaxed particles during specimen preparation.

3:00 PM

(ENERGY-074-2010) Durability Testing of Glasses for the Stabilization of Closed Nuclear Fuel Cycle Waste Streams

A. L. Billings*, J. C. Marra, Savannah River National Laboratory, United States; J. V. Ryan, J. D. Vienna, J. V. Crum, Pacific Northwest National Laboratory, United States; C. S. Ray, Mo-Sci, United States

The Fuel Cycle Research and Development (FCR&D) program is sponsored by the US DOE to develop and demonstrate a process for the recycling of spent nuclear fuel in order to achieve a closed nuclear fuel cycle. Borosilicate glass was selected as the baseline technology for immobilization of the Cs/Sr/Ba/Rb, lanthanide and transition metal fission product waste steams. However, additional glass compositions (e.g. iron phosphate glasses) glass-ceramic and ceramic waste forms are now being considered for this combined waste stream. Immobilization of the combined waste streams has several advantages; namely minimization of the number of waste forms and waste form processes, and a minimization of waste handling steps. A joint study was undertaken by Pacific Northwest National Laboratory and Savannah River National Laboratory to develop acceptable borosilicate glasses for the various waste streams. Concurrently, researchers at the Missouri University of Science and Technology developed iron phosphate glasses for the combined waste stream. These studies were aimed to develop and test glasses which could successfully immobilize the waste streams and have acceptable chemical durability. Product Consistency Testing (PCT) and chemical composition analyses on all glasses from these studies were conducted so key waste components and their impact on waste loading and durability could be identified.

3:40 PM

(ENERGY-075-2010) Development of Iodine Waste Forms Using Low-Temperature Sintering Glass

T. Garino*, T. Nenoff, J. Krumhansl, D. Rademacher, Sandia National Laboratories, United States

This presentation will describe our recent work on the use of low temperature-sintering glass powders mixed with either AgI or AgI-zeolite to produce a stable waste form. Radioactive iodine (^{129}I, half-life of 1.6×10^{7} years) is generated in the nuclear fuel cycle and is of particular concern due to its extremely long half-life and its effects on human health. As part of the DOE/NE Advanced Fuel Cycle Initiative (AFCI), the separation of ^{129}I from spent fuel during fuel reprocessing is being studied. In the spent fuel reprocessing scheme under consideration, the iodine is released in gaseous form and collected using Ag-loaded zeolites, to form AgI. Although AgI has extremely low solubility in water, it has a relatively high vapor pressure at moderate temperatures (>550°C), thus limiting the thermal processing. Because of this, immobilization using borosilicate glass is not feasible. Therefore, a bismuth oxide-based glasses are being studied due to the low solubility of bismuth oxide in aqueous solution at pH>7. These waste forms were processed at 500°C, where AgI volatility is low but the glass powder is able to first densify by viscous sintering and then crystallize. Since the glass is not melted, a more chemically stable glass can be used. The AgI-glass mixture was found to have high iodine leach resistance in these initial studies.

4:00 PM

(ENERGY-076-2010) Cermet High-Level Waste Forms

R. T. Jubin*, W. S. Aaron, E. D. Collins, V. F. De Almeida, G. D. DelCul, D. W. DePaoli, L. K. Felker, B. D. Patton, S. L. Voit, Oak Ridge National Lab, United States

The successful re-expansion of nuclear energy is dependent on the development of waste disposal options that minimize repository use and maximize efficiency and public safety. Work is currently underway at ORNL to develop an advanced cermet waste form concept for the optimal storage of high-level wastes generated in used nuclear fuel treatment. Cermets are composed of ceramic phases dispersed in continuous metal matrices. This provides an opportunity to tailor the primary phases to take optimal advantage of the properties of both metallic and oxide materials. This paper will describe two aspects of this effort. We will discuss the efforts to fabricate and characterize the cermet materials containing very high mass fractions of fission product waste materials from the recycle of used nuclear fuels. The materials produced to date have been formed with minimal additives thus maximizing the fission / activation product content of the final waste form. We will also discuss the efforts directed toward the modeling of the resulting cermet materials. This will cover both the methods and modeling tools needed to analyze the formation and performance of the resultant materials in terms of chemical thermodynamics and heat transfer.

4:20 PM

(ENERGY-077-2010) Functionalized silica aerogels for capturing and immobilization of I, Kr, and CO2

J. Matyas*, G. E. Fryxell, K. Wallace, L. S. Fifield, Pacific Northwest National Laboratory, United States

Release of radiological off-gas into the atmosphere will no longer be acceptable during the reprocessing of spent nuclear fuel. The U.S. Environmental Protection Agency requires the gaseous radionuclides such as 129I, 85Kr, and 14C (as 14CO2) captured to meet a goal of limited emissions and immobilized to meet the disposal restriction regulations for radioactive waste. The chemically modified silica aerogel materials were developed at PNNL that can effectively capture and dispose iodine, krypton, and carbon dioxide. The surfaces of silica aerogels were chemically modified with the supercritical fluid chemistry. The success of surface functionalization and high gas sorption capacity of functionalized silica aerogels were investigated with an array of experimental techniques. The raw and gas-loaded aerogels were densified by thermal sintering with pressure assistance. The retention of gases in sintered aerogels was quantified by chemical analysis. This work has shown that it is possible to functionalize silica aerogels (something that is difficult to do using traditional solvent-based methods due to the frailty of the aerogel backbone), that these functionalized aerogels can be effective for capturing a variety of airborne target species, and that once laden with contaminants these materials can be sintered/densified, creating a stable composite that could be a viable waste form.

4:40 PM

(ENERGY-078-2010) New Generation Nuclear Waste Forms Based on Nano-Encapsulation

Y. Wang*, Sandia National Laboratories, United States

Development of durable waste forms for disposition of various waste streams generated in spent fuel reprocessing is technically challenging. I here present a new concept for the development of waste forms based on nano-encapsulation of radionuclides. The new type of waste forms are made in two steps: synthesizing nanoporous radionuclide-getter materials and converting these materials into durable nanocomposites. Nanoporous alumina and its derivatives are found to have high sorption capabilities various radionuclides (e.g. I-129). These materials are synthesized with sol-gel routes using inexpensive inorganic precursors. Radionuclides sorbed inside the nanopores of these materials are immobilized through precipitation or other chemical transformations. The radionuclide-loaded materials are finally mixed with glass-forming frits and calcined at appropriate temperatures to form glass-ceramic composites, in which nanometer radionuclide precipitates are encapsulated in a glass or crystalline matrix. The new waste forms developed as such have several significant advantages. Unlike the traditional ones, which tend to incorporate radionuclides into rigid crystal structures, the new waste forms incorporate radionuclides as nano-scale inclusions in a host matrix. The resulting waste forms can accommodate a wide spectrum of radionuclides with high waste loadings and low leaching rates.

Poster Session

Room: Horizons

(ENERGY-P001-2010) Electrochemical Behaviour of Palladium Nanoparticles as Catalysts for Direct Formic Acid Fuel Cells (DFAFC)

M. Balandeh*, D. Buckley, University of Limerick, Ireland

Polymer electrolyte membrane (PEM)-based fuel cells are generally considered as variable candidates to replace batteries in portable power devices. It is the limitations of hydrogen and methanol that have in recent years increased interest in direct formic acid fuel cells (DFAFCs). Various Platinum and palladium based catalysts have been extensively studied for the electrocatalytic oxidation of formic acid. Recent studies have shown that palladium is an efficient catalyst for formic acid oxidation to CO2 through a direct pathway, and thereby yield high performance in a DFAFC. In this work unsupported Palladium nanoparticles were prepared by a chemical reduction method, and characterized by a wide array of experimental techniques including scanning electron microscopy, X-ray diffraction spectroscopy and particle size analyzer. Meanwhile, the electrocatalytic activity of Pd electrodes for formic acid oxidation is studied. It is found that the obtained nanoparticles exhibit excellent catalytic activity for formic acid electrooxidation.

(ENERGY-P002-2010) High Performance Nanofluids with Encapsulated Phase Change Nanoparticles for Energy Storage and Heat Transfer

Y. Hong*, W. Wu, S. Ding, L. Chow, M. Su, University of Central Florida, United States

We report the encapsulation of phase change metallic nanoparticles using non-melting and non-conductive shells to enhance the heat capacity and thermal conductivity, and preserve the dielectric property of cooling fluid. The encapsulated nanoparticles are made at high production yield by boiling powders of metals or alloys in liquids that have high boiling temperatures, followed by shell formation using sol-gel method. Transmission electron microscopy (TEM) has confirmed the core-shell structures of encapsulated phase change nanoparticles. The thermophysical properties of nanofluids are measured by using differential scanning calorimetry (DSC) and using a heat transfer loop. The frequency dependent dielectric measurements of base fluid PAO, PAO with bare nanoparticles (In/PAO), and PAO with silica encapsulated nanoparticles (In@SiO2/PAO) have confirmed the effects of encapsulation. The innovative points of this work include: (1) the dielectric encapsulation of nanoparticles allows the direct immersion cooling of electronics; (2) non-melting shell prevents aggregation of molten nanoparticles; (3) the direct boiling of alloys allows the synthesis of alloy nanoparticles with different melting temperature; and (4) the high yield production of encapsulated metallic nanoparticles for large scale applications.

(ENERGY-P003-2010) Fabrication and characteristics of Li-Ti-O thin film for solid state thin film supercapacitor(TFSC)

S. Kim*, Y. Yoon, Yonsei University, Korea, Republic of

lithium titanium oxide (Li-Ti-O) material has been focused on as a superior electrode for supercapacitor. The Li-Ti-O material has advantages that include its flat electrical potential, proper working voltage, good capacity, extended cycle life. Li-Ti-O thin films prepared by sol-gel process for electrode had been reported. However, this process is not good for in-situ based process. In this study, Li-Ti-O thin films were deposited using a RF reactive magnetron sputtering method at room temperature with various working pressure of pure Ar (5, 10, 50 mtorr). Effects of working pressure and plasma immersion during sputtering process on the electrochemical and structural properties of Li-Ti-O thin films were investigated in order to reveal possibility for sputter grown Li-Ti-O thin film as electrode of all solid state TFSC. Comparing with working pressure and plasma immersion effects, structural and electrochemical properties of the as-deposited Li-Ti-O thin films depended strongly on the plasma immersion. In addition, electrochemical behavior such as capacity could be improved by the plasma immersion. These results indicated that better electrochemical behavior of all solid state TFSC could be achieved by plasma immersion deposition of Li-Ti-O thin film even at room temperature.

(ENERGY-P004-2010) Synthesis and Characterization of Nanostructured ZnCo2O4/Co2O3 for Electrochemical Supercapacitors

O. Dominguez*, Instituto de Metalurgia UASLP, Mexico; L. M. Flores-Velez, Facultad de Quimica UASLP, Mexico; R. Cruz, Instituto de Metalurgia UASLP, Mexico; R. Martinez, I. Esparza, CIMAV, Mexico

Electrochemical supercapacitors are investigated due to their interesting characteristics in terms of power and energy densities. Here we present preliminary results of ZnCo2O4/Co2O3 as active materials for electrochemical supercapacitors. The active nanostructured material was synthesized using Zn/Co salts dissolved in water at 60 °C. Triethanolamine with drops of a NH4OH solution were added and stirred. The as-prepared powders were treated at 200 °C to obtain the nanostructured ZnCo2O4/Co2O3 with mean particles sizes of 5 nm. Composite electrodes were prepared by mixing the active material with carbon black and pressed at 900 MPa on a stainless steel grid. The crystalline structure was examined using X-ray Diffraction and decomposition was observed using a thermogravimetric analyzer. The morphology of the samples was investigated by transmission electron microscopy. For cyclic voltammetry, an electrochemical analyzer was used with a module to carry out impedance spectroscopy. From Nyquist plot, it was estimated a charge transfer resistance for the electrode of 10 ohms and from the cyclic voltametry at 5 mV/s, the specific capacitance shifted from 60 to 100 F/g as the ratio of ZnCo2O4/Co2O3 was modified. Therefore this composite material could be an economic electrode material with good specific capacitance and low impedance if long cyclic life could be obtained.

(ENERGY-P005-2010) Advanced assessment of batteries, fuel cells & their materials using gas sorption, calorimetry and thermal analysis

A. Levchenko*, Setaram Inc, United States

The new materials developed in the recent years in the field of batteries and fuel cells present a number of challenges to the research community from a viewpoint of materials characterization. Calorimetry and thermal analysis have been regarded as essential tools in assessment of materials performance and properties including applications such as hydrogen storage materials, fuel cells, batteries and battery materials. We have recently employed the advanced gas sorption and calorimetric techniques for characterization of hydrogen storage materials and for CO2 capture and sequestration applications. In this paper we will also present calorimetric characterization techniques of batteries, cells and their materials ranges from screening materials, to self discharge and of course abuse and overcharge testing.

(ENERGY-P006-2010) Sintered clay waste form for immobilization of cesium and strontium liquid waste

L. H. Ortega*, Texas A&M University, United States; M. D. Kaminski, Argonne National Laboratory, United States; S. M. McDeavitt, Texas A&M University, United States

In order to reduce the heat output from spent nuclear fuel, the Advanced Fuel Cycle Initiative proposed separating and stabilizing a concentrated stream of cesium and strontium. We prepared a simulated waste solution by dissolving nitrate salts of cesium, strontium, barium, and rubidium into a dilute nitric acid. The simulated waste was mixed with natural bentonite clay, dried, axially pressed, and then sintered at various temperatures. Neutron activation analysis determined total waste concentrations of 32 wt%. X-ray diffraction analysis found pollucite and monoclinic feldspars of barium and strontium had formed. The mineral phases were segregated by oxidation state, observed with scanning electron microscopy, and wave dispersive analysis. Leach rates were analyzed by the TCLP test. Sintering above 1100°C was necessary for adequate strontium immobilization. The bentonite clay provided alumina and silica, which reacted with the alkaline and alkali earth metals during sintering. The process formed a hard multi-phase ceramic. The immobilization of alkali and alkaline earth metals in sintered bentonite clay may provide a relatively simple alternative to vitrification or engineered sequestration agents.

(ENERGY-P007-2010) Radiation damage effects in multi-layer thin film MgO/HfO_2 structures

I. Usov*, J. Won, J. A. Valdez, M. Hawley, D. J. Devlin, R. M. Dickerson, G. D. Jarvinen, K. E. Sickafus, Los Alamos National Laboratory, United States

One of the promising directions in the development of new nuclear fuel forms is a transition from traditional single phase fuels such as UO_2 to fuel elements consisting of at least two phases: fissile and non-fissile. For this study we fabricated a multi-layer structure composed of MgO (non-fissile) and HfO_2 (fissile component surrogate) thin films. The goal of this study was to investigate radiation damage induced microstructural evolution (TEM, GIXRD) and intermixing (STEM, RBS) under irradiation conditions simulating nuclear fuel environment. The multi-layer structures were irradiated with 10 MeV Au ions over a wide range of fluencies (from $5x10^{13}$ to $3.7x10^{16}$ Au/cm^2). We observed in the multi-layer structures radiation effects typical of its individual components, such as absence of amorphization in both MgO and HfO_2 layers and phase transformation from monoclinic to tetragonal HfO_2 polymorphs. In addition, formation of voids at the MgO/HfO_2 interface was revealed, which is not characteristic to either material exposed to ion irradiation. Dramatic structural changes (crack healing and large craters) were also observed on the surfaces of the multi-layer samples. Our conclusion is that radiation effects in composites, consisting of dissimilar materials, are not always derived simply from their individual components and therefore, radiation effects in composites need to be investigated separately.

(ENERGY-P008-2010) Fabrication and Property Relations of Transuranic Actinide Containing Ceramic Oxides

S. P. Willson*, Los Alamos National Laboratory, United States

Americium and neptunium are long-lived fission products present in spent nuclear fuel that contribute substantially to the radiotoxicity of a spent fuel repository. One approach to reducing the hazards of nuclear waste and closing the nuclear fuel cycle is incorporation of these elements into a new fuel form and transmutation in a nuclear reactor. Mixed uranium/plutonium oxide (MOX) fuel is a common ceramic fuel type and therefore is a logical reference for development of a minor actinide bearing fuel. Incorporation of the minor actinides neptunium and americium into existing uranium/plutonium mixed oxide (MA-MOX) fuel forms necessitates nontrivial changes in the fabrication process and results in differences in properties of sintered fuel pellets relative to conventional MOX. Critical challenges for MA-MOX development include understanding and controlling the relationships between feed powder characteristics, fabrication processes and corresponding fuel properties. This talk will present progress to date on establishing those relationships for development of MA-MOX fuel for minor actinide transmutation in a fast reactor.

(ENERGY-P009-2010) Effects of Oxygen to Metal Ratios in High Burn-up Actinide Ceramic Oxides

J. T. Dunwoody*, S. P. Willson, D. D. Byler, K. J. McClellan, R. E. Mason, M. R. Lopez, D. R. Martinez, A. C. Martinez, Los Alamos National Laboratory, United States

Transmutation of long-lived minor actinides such as americium, neptunium and possibly curium, is being considered as a path to reducing the radiotoxicity of spent nuclear fuel material requiring long-term storage in a geologic repository. Minor actinide bearing mixed oxide fuel (MA-MOX) may serve as a transmutation fuel form. The utilization of conventional plutonium and uranium mixed oxide (MOX) as fuel for fast spectrum reactors has been well documented, and the effects of O/M on such considerations a burn-up, fuel melting point, and fuel/cladding chemical interactions (FCCI) are pertinent to the design of these transmutation oxides. MA-MOX designed to achieve high burn-up would necessarily require lower starting oxygen to metal (O/M) ratios, due to the effects of excess oxygen on fuel melting point and FCCI. Controlling the O/M during fabrication of MA-MOX fuel and understanding the relationship between oxygen stoichiometry, fuel properties, and corresponding fuel performance is an important aspect of MA-MOX fuel development. Recent results from development of MA-MOX for fast reactor transmutation will be presented and referenced to analogous MOX compositions.

(ENERGY-P010-2010) Utilization of Pondash in Highway Engineering

R. Sarkar, A. Varma*, A. Garg, M. Saxena, P. Sharma, N. Khanna, Delhi College of Engineering, India

India is now regarded as a potential leader in technical sector. However with rise in development of sophisticated technology there has been a parallel and exponential increase in demand of power and electricity. India has long been tapping energy from thermal power, leading to tremendous production of coal ash. It has hitherto been considered as a waste material, but now various ways to fruitfully utilize this by-product have been designed. An effort has been done to employ pond ash, combined with varying percentages of bentonite, as a prospective resource in highway engineering. California Bearing Test (CBR) is performed on samples of pond ash along with certain amount of bentonite and the results hence obtained are analyzed and inferences are drawn. The most evident conclusion drawn, from the graphs plotted on the basis of figures obtained from the CBR tests, is that with increase in percentage of bentonite, which happens to be a type of fine clay, the load bearing capacity of the pond ash sample decreases. This can be comprehended from the fact that CBR values obtained keep on decreasing with subsequent increase in percentage of bentonite. Keywords : Pond ash, Bentonite, California Bearing Test(CBR)

(ENERGY-P011-2010) The performances of ceramic based membranes for fuel cells

U. Thanganathan*, Okayama University, Japan

These days' environmental issues due to increases in emissions of air pollutants and greenhouse gases are driving the development of clean

energy delivery technologies such as fuel cells. Low temperature proton exchange membrane fuel cells (PEMFC) use hydrogen as a fuel and their only emission is water. In addition to high proton conductivities, these materials have demonstrated chemical stabilities, and can thus potentially substitute organic compounds as electrolytes. The proton transport mechanism in a composite electrolyte consists of a surface and bulk mechanisms that are mainly associated with the functional groups and the pore channels, respectively. The conduction of protons in the composite membranes was mainly due to the hopping of protons through the hydrogen bonded water and hydroxyl groups in the network structure, or in other words, the protons were transported on the surfaces of the pore channels. The content of protons in inorganic/organic composites decreases with an increase in the sintering temperature of the membrane. Therefore, it is desirable to prepare the inorganic/organic composite membrane with a large amount of protons at low temperature.

(ENERGY-P012-2010) Kinetics of H2 Desorption from TiN-Destabilized NaAlH4

W. D. Ukpai*, S. Narase Gowda, T. A. Dobbins, Louisiana Tech University, United States

This project is designed to extend the limits of hydrogen storage technology for practical purposes. Currently, there is a need to develop systems which release hydrogen at lower temperatures. Addition of destabilizers (such as TiN) will lower the H2 gas desorption temperatures from NaAlH4 by forming a stable Ti-Al alloy. Sodium alanate powders were destabilized using titanium nitride (TiN) using varying concentrations of TiN, 25 mol%, 50 mol%, and 75 mol%. The kinetics of the H2 desorption reaction were studied using mass spectrometry. The formation of TiAl in the destabilized system was confirmed by X-ray diffraction. Desorption temperatures were reduced from 180C to 125C in these powders. Mass Spectrometry was used to examine the elemental composition of the samples at various desorption temperatures.

(ENERGY-P013-2010) Empirical Method to Estimate Hydrogen Embrittlement of Metals as a Function of Hydrogen Gas Pressure at Constant Temperature

J. A. Lee*, NASA-Marshall Space Flight Center, United States

High pressure Hydrogen gas has been known to have a deleterious effect on the mechanical properties of certain metals, particularly, the notched tensile strength, fracture toughness and ductility. The ratio of these properties in Hydrogen as compared to Helium or Air is called the Hydrogen Environment Embrittlement (HEE) Index, which is a useful method to classify the severity of H embrittlement and to aid in the material screening and selection for safety usage H gas environment. A comprehensive NASA and world-wide database compilation, in the past 50 years, has shown that the HEE index is mostly collected at two convenient H pressure points of 5 ksi and 10 ksi near room temperature. Since H embrittlement is directly related to pressure, the lack of HEE index at other pressure points has posed a technical problem for the designers to select appropriate materials at a specific H pressure for various applications in aerospace, alternate and renewable energy sector for an emerging hydrogen economy. An empirical method to accurately estimate the HEE index, as a function of H pressure at constant temperature, is presented with a brief review on Sievert's law for gas-metal absorption.

(ENERGY-P014-2010) Ultrasmall Angle X-ray Scattering (USAXS) Studies of Mophological Changes in NaAlH4

S. Narase Gowda*, T. A. Dobbins, Louisiana Tech University, United States

Ultra Small Angle X-Ray Scattering (USAXS) technique has been explored to study morphological changes that occur in the hydrides during various stages of hydrogen release. The power law scattering data [intensity(I) vs. scattering wave vector(Q)] from USAXS measurements yield the power law slope (p) which is used as a definitive parameter to study changes in surface fractal dimensions (Ds). Changes in surface area occur because of densification during desorption at elevated temperatures and the rate of those changes in surface area are mitigated by the addition of transition metal dopants. For the present study, NaAlH4 was doped with 4 mol% TiCl3 by high energy ball milling and were subjected to USAXS measurements to study the effect of the catalyst. Doped and undoped NaAlH4 were also nano-confined within porous alumina membranes and tested for effects of nano-confinement. Results showed that the surface area of the particles decreased after catalyst addition. This decrease in surface area can be attributed to the densification because the hydride experiences elevated temperatures during high energy milling.

(ENERGY-P015-2010) Ammonium borohydride: Solid Hydrogen Storage Material with Highest Gravimetric Hydrogen Content

A. Karkamkar*, D. Heldebrant, J. Linehan, T. Autrey, Pacific Northwest National Lab, United States

Various options for hydrogen storage are being studied ranging gases (hydrogen), liquids (e.g., methanol) to solids (e.g., lithium borohydride, boranes and amides). However, no single material today meets all the required technical targets. Here we report the synthesis, structure and hydrogen desorption properties of a unique hydrogen storage material, i.e., one that stores hydrogen on both the cation and anion, ammonium borohydride. Further we show the compound releases greater than 20 wt% hydrogen in three steps at temperatures less than 180 °C and provide evidence that NH4BH4 crystallizes at room temperature and standard pressure in a rock-salt structure. The experimental lattice parameters provide an estimate of the volumetric density, ca. 154 g Hydrogen/liter of NH4BH4. The high volumetric capacity is comparable to many metal hydrides, however, as NH4BH4 has hydrogen stored on both the cationic and anionic sites which leads to a significantly greater gravimetric density (244 gm Hydrogen/kg).

(ENERGY-P016-2010) Performance Evaluation of Oxide Catalyst-doped Ni-Zirconia and Ni-Ceria based Anodes for Methane Fueled SOFCs

J. Myung*, J. Lee, S. Hyun, Yonsei University, Korea, Republic of

Solid oxide fuel cells (SOFCs) with low emissions and high-energy conversion efficiency can directly use hydrocarbon fuels without use of a reformer. Conventional Ni-based cermet anodes have commonly been used as an anode material with catalytic properties for hydrocarbon fuel. However, carbon deposition is a critical problem which causes loss of cell performance and poor long-term stability during internal reforming. We have focused on the development of oxide catalysts such as Li2TiO3 and evaluated the performance of catalyst-doped anode supported SOFCs for methane fuel. The Li2TiO3 catalyst could be synthesized by the solid state reaction method and the catalyst-doped Ni-YSZ anodes reduced the amount of carbon deposition by 80% compared with the original Ni-YSZ anodes. The catalyst (Li2TIO3)-doped Ni-YSZ/Ni-GDC anode supported YSZ/GDC electrolytes were manufactured by die-pressing the Ni-YSZ-Li2TiO3/Ni-GDC-Li2TiO3 powder mixture, followed by dip-coating YSZ/GDC electrolyte slurry on die-pressed anodes. The final catalyst-doped anode supported unit cells were prepared by screen-printing LSM-YSZ/LSCF-GDC paste on the electrolyte layer. Both Li2TiO3 catalyst-doped Ni-YSZ and Ni-GDC anodes showed sufficient electrical conductivity and porosity as an anode. The power density of the catalyst-doped Ni-YSZ anode supported unit cells showed more than 0.4 W/cm2 at 800°C, and their long-term stability was considerably improved for CH4 fuels. Moreover, the power density and long-term stability of these cells could be greatly enhanced by inserting a Li2TiO3 catalyst-doped functional layer between anode and electrolyte.

(ENERGY-P017-2010) Carbon Building Materials from Coal Char: Durable Materials for Solid Carbon Sequestration

J. Halloran*, University of Michigan, United States

The pyrolysis of coal can produce clean fuels, such as hydrogen-rich gases and liquid hydrocarbons. It also produces coke-like coal char. Rather than using the coal char as a fuel, it can be used the basis of carbon building materials (CBM) which sequester the carbon in the solid state while performing an essential function. Data is presented on the properties of prototype of coal-char based solid carbon, which is stronger and lighter than conventional concrete or fired clay masonry. We present analyses on the economic viability for co-production of hydrogen fuels and CBM from coal. We analyze the environmental benefits of substituting CBM for Portland cement-based concrete products in terms of carbon dioxide emissions and land spoilage. We show that solid sequestration of pyrolysis char as building materials provides green energy from coal.

(ENERGY-P018-2010) Environmental Catalysts from Biochar

J. Kastner*, University of Georgia, United States; P. Kolar, North Carolina State University, United States; A. Teja, Georgia Tech, United States

Biomass can be pyrolyzed to generate a bio-oil as a potential liquid fuel and a solid char. The resultant char can form the basis of carbon supported catalysts, providing additional value added products from the biorefinery. Char can be further combusted to generate power and heat, but results in an ash that is typically landfilled. However, the resultant materials hold promise as industrial catalysts. Ash and carbon supported catalysts generated from char would have several distinct advantages over alumina or silca supported systems, yet little research has focused on using these materials as catalysts. Traditional methods of solid catalyst preparation limit control of key variables in catalyst design and thus limit activity and selectivity. Recent advances in the synthesis of nanocrystalline materials have allowed for generation of advanced catalytic material with better control over key variables such as dispersion, shape, size, crystal composition and structure, and surface area. We have demonstrated the use of electrochemical deposition of metals on activated carbon (similar to electroplating) at room temperature as a green method of making carbon supported catalysts from char. We will present research results on the use of wood ash, biomass char, metal oxide nano-particle impregnated char and electrochemically metal deposited char as catalysts for the room temperature oxidation of ammonia and low molecular weight aldehydes (VOCs).

(ENERGY-P019-2010) Superhydrophobic membrane distillation for water desalination

M. Su, University of Central Florida, United States; Z. Ma*, Y. Hong, L. Ma, Unversity of Central Florida, United States

Membrane distillation desalinates seawater using low-grade heat energy or solar heat, but this method has low mass fluxes and membrane fouling issues. The random microstructures of existing polymeric membranes have torturous microstructures and large diffusion resistance for water vapor and will be easily contaminated by particulates contained in water. We have made superhydrophobic membranes by glass fiber-drawing and investigated the effects of membrane microstructures on water desalination. Novel glass membranes with integrated arrays of nanospiked microchannels and sharp pore size distribution have been produced at high yield using a process that involves glass fiber drawing, dissolving template material, and differential chemical etching. Such superhydrophobic membranes have shown better performance than those of existing polymer membranes in terms of water fluxes and antifouling properties especially at high salt concentration. The high desalination performance is believed to be the result of the membrane's large pore diameter, straight pore shape, narrow pore size distribution, excellent water-repelling property and superior chemical and thermal stabilities. This superhydrophobic membrane can be potentially used for solar energy-driven water desalinations to replace expensive electric-driven osmosis in remote areas.

(ENERGY-P020-2010) On enhancing efficiency of dye-sensitized solar cells by MPII-implanted ruthenium ions

D. Wang, MingDao University, Taiwan; C. Yen*, National Chung Hsing University, Taiwan; M. Shih, MingDao University, Taiwan; L. Chang, National Chung Hsing University, Taiwan; H. Shih, Chinese Culture University, Taiwan

The dye-sensitized solar cells (DSSC), which are based on the concept of photosensitization of wide band gap mesoporous oxide semiconductors, are now in the state of advanced development and pilot production. Our current research emphasizes on the improvement of the photosensitivity of TiO2 under visible light irradiation by using metal plasma ion implantation technique (MPII). The nano-crystalline TiO2 electrode was prepared by a sol-gel process and deposited on ITO glass substrates. Subsequently, the as-deposited TiO2 films were subjected to MPII at 20 keV to incorporate transition metals of Ru surface. In this study, we will investigate the corelation between the Ru implantation and the photovoltaic behaviors of TiO2 DSSC under a simulated Am 1.5 solar light irradiation. The composition and chemical bonding of the doped dye-sensitized solar cells were evaluated by X-ray photoelectron spectroscopy. An UV/visible spectroscope were used for the energy band gap measurement to assess the performance of the metal-implanted dye-sensitized TiO2 for solar cell applications.

(ENERGY-P021-2010) Spin-engineered suppression of dominant non-radiative shunt paths in Ga(In)NAs relevant to photovoltaic applications

X. J. Wang, Y. Puttisong, Linköping University, Sweden; C. W. Tu, University of California, United States; A. J. Ptak, National Renewable Energy Laboratory, United States; V. K. Kalevich, A. Y. Egorov, A F Ioffe Physico-Technical Institute, Russian Federation; L. Geelhaar, H. Riechert, Paul-Drude-Institut für Festkörpelektronik, Germany; I. A. Buyanova, W. M. Chen*, Linköping University, Sweden

Ga(In)NAs dilute nitrides hold potentials for photovoltaic applications such as highly efficient multi-junction solar cells. Unfortunately, developments of these devices have largely been hindered by introduction of defects, which provide efficient non-radiative shunt paths for photo-generated carriers. Here we identify Ga interstitials as the dominant non-radiative defects in Ga(In)NAs. At least three different types of Ga interstitial defects can be distinguished based on their hyperfine structures. Their formation is shown to strongly depend on growth methods and conditions, as well as post-growth rapid thermal annealing. Defect concentrations are found to increase with increasing N composition and with decreasing growth temperature. The carrier recombination process via these defects is discovered to be strongly spin-dependent, which allows efficient spin-blockade of such process. This spin blockade results in a significant improvement in non-equilibrium carrier lifetime, leading to a drastic increase by up to 800% in efficiency of photo-generation. As these defects seem to be unavoidable with the current growth technologies, the demonstrated spin blockade appears to offer an attractive strategy to strongly suppress non-radiative shunt paths harmful to photovoltaic devices.

(ENERGY-P022-2010) The Potential of Fiber Optimization for Transport of Solar Radiations

J. Wang*, National Sun Yat-Sen University, Taiwan

Transporting solar energy by optical fiber provides many unique advantages, such as design flexibility and reliability of receiver, and potentially promotes other novel applications and improvements of solar energy utilization. For instance, in the case of solar-thermal application, delivering radiations in fiber at infrared spectra are more efficient and desired. The advance of fiber development has been excellent with respect to both fiber quality and functionality of specialty optical fibers. However, these fibers were mainly focusing on the application of optical fiber communications. Therefore, it is worthy to specifically develop a new class of transmission fibers for solar radiations since the great demand of green energy around the world. In order to extend the full potential of fibers for energy application, I would study the fibers from both physical and material prospects. A transmission comparison of solar radiation in conventional multimode fibers, microstructured optical fibers and double clad fibers will be investigated. The advantages and disadvantages of fibers made from different hosts would be discussed with respect to specific applications. For instance, a fiber having low phonon energy may improve the lifetime of fiber for delivery of intense solar energy. Ultimately, optimal designs of fiber for solar energy transmission will be presented and discussed.

(ENERGY-P023-2010) Cu2ZnSnSe4 thin films produced by selenization of Cu-Zn-Sn containing precursor films

O. Volobujeva*, E. Mellikov, S. Bereznev, J. Raudoja, Tallinn University of Technology, Estonia

Thin film solar cells based on different stannite adsorber films are perspective candidates for large scale solar energetics. In this study, the evolution of surface morphology, phase composition and homogeneity of CZTS (Cu2ZnSnSe4) in selenization process of precursor metallic and binary stacked films is studied using high resolution SEM, micro-Raman, XRD, XRF, EBSD and EDS techniques. It was shown that surface morphology of selenized films depends strongly from composition (staked metallic, binary) and sequence of layers in precursor films. Additionally the phase composition and structure of Cu2ZnSnSe4 films produced by the selenization of precursors in Se atmosphere in dependence of nature and sequence of consistent layers in precursor films will discussed.

Wednesday, February 24, 2010

Hydrogen

Nanostructures and Catalytic Materials for Hydrogen Storage

Room: Seashore Ballroom

Session Chairs: Rana Mohtadi, Toyota Research Institute of North America; Gavin Walker, University of Nottingham

8:00 AM

(ENERGY-079-2010) Savannah River National Laboratory Regenerative Fuel Cell Project

T. Motyka*, Savannah River National Laboratory, United States

A team comprised of governmental, academic and industrial partners led by the Savannah River National Laboratory developed and demonstrated a regenerative fuel cell system for backup power applications. Recent market assessments have identified emergency response and telecommunication applications as promising near-term markets for fuel cell backup power systems. The Regenerative Fuel Cell System (RFC) consisted of a 2 kg-per-day electrolyzer, metal-hydride hydrogen storage units and a 5 kW fuel cell. Coupling these components together created a system that can produce and store its own energy from the power grid much like a rechargeable battery. A series of test were conducted to evaluate the performance of the RFC system under both steady-state and transit conditions that might be encountered in typical backup power applications. In almost all cases the RFC functioned effectively. Test results from the demonstration project will be used to support recommendations for future component and system designs and support potential commercialization activities. Further testing of the RFC system at the Center for Hydrogen Research in Aiken County, SC is being planned. These plans include evaluating the system as a renewable system coupled with a 20kW-peak solar photovoltaic array. This paper will discuss recent results from the RFC testing along with future plans for the system.

8:20 AM

(ENERGY-080-2010) Novel high temperature proton conducting polymer electrolyte membrane

J. Iroh*, W. Lu, J. Wang, University of Cincinnati, United States

One class of polymers that is being evaluated for use in producing high temperature proton conducting polymer electrolyte membrane, PEM is (poly(arylene(1,3-imidazolelidine-2,4,5-trione-1,3-diyl)), commonly known as polyparabanic acid, PPA. PPA has a rigid and stiff backbone, a high glass transition temperature, Tg > 160C and high proton conductivity of about 2 x 10-2 Scm-1 at 160C. PPA homopolymer and block copolymers have been successfully synthesized in our laboratory. Advanced analytical techniques such as scanning electron microscopy, SEM, and Fourier transform infrared spectroscopy, FTIR, were used to determine the structure and composition of the copolymers. The transition temperature and decomposition temperature for the polymers were determined by using differential scanning calorimetry, DSC and thermogravimetric analyzer, TGA. The electrochemical property of the solution cast membranes was measured by using electrochemical impedance spectroscopy, EIS. Our preliminary results show that the conductivity of the membrane increased by more than three orders of magnitude after doping with appropriate doping agent.

8:40 AM

(ENERGY-081-2010) Fabrication of Palladium Coated Nanoporous Carbon Nanofibers via Electrospinning

H. Kim*, Yonsei University, Korea, Republic of; D. Lee, Yonsei University, Korea, Republic of; J. Moon, Yonsei University, Korea, Republic of

Electrospinning is a technique that produces sub-micron sized continuous fibers by electric force from polymer solution or melt. Due to the versatile manufacturability and cost effectiveness, this method has been recently adopted for the fabrication of one-dimensional materials. Here, we fabricated polyacrylonitrile (PAN) fibers from which uniform carbon fibers with the diameter 100-200 nm were obtained after carbonization at 800oC in H2O+N2. In particular, PAN nanofiber was fabricated by electrospinning using two different polymer solutions. PAN was located in the sheath of the fiber, whereas poly(styrene-co-acrylonitile) (SAN) was positioned at the center of the fiber. Palladium solution was also electrosprayed on the surface of electrospun fibers in order to improve the hydrogen storability. After the reduction and carbonization, we obtained the nanosized Pd coated carbon fibers. The coated Pd had the average particle size in the range of 10~50 nm, exhibiting a uniform surface coverage. The morphologies and the microstructure were observed by SEM and TEM. XPS and Raman spectroscopy were also used to identify the surface composition and the degree of carbonization. Hydrogen adsorption kinetic curves were measured to determine the hydrogen contents and pressure–composition isotherm was evaluated at different temperature to reveal hydrogenation/dehydrogenation properties of carbon nanofiber.

9:00 AM

(ENERGY-082-2010) Nanostructured Platinum for Fuel Cells

F. van Swol*, Y. Song, M. A. Hickner, Sandia National Laboratories, United States; S. R. Challa, R. M. Garcia, H. Wang, C. J. Medforth, University of New Mexico, United States; J. E. Miller, J. A. Shelnutt, Sandia National Laboratories, United States

We have developed an innovative nanotechnology for producing platinum catalysts that offers much greater control over the shape, size, porosity, composition, stability, and other functional properties of platinum nanostructures than those achieved by existing methodologies. Novel catalysts and electrocatalysts produced by this approach are expected to reduce the platinum metal usage and thus the cost of platinum catalysts for use in fuel cells, solar cells, and other applications in the renewable energy sector. Some of the platinum nanostructures also exhibit enhanced structural durability to ripening processes, thereby preserving the high surface area and activity of catalysts in a range of technologically and industrially important processes. Under electron-beam irradiation, dendritic platinum nanosheets structurally evolve into metastable “holey” nanosheets. Monte Carlo simulations of this structural transformation agree well with electron microscope images detailing the ripening process. The experiments and simulations show that nanoscale holes of a critical size are persistent and give holey sheets their morphological stability, sustained high surface area, and remarkable ripening resistance. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DEAC04-94AL85000.

9:20 AM

(ENERGY-083-2010) Novel Hydrogen Storage Properties Derived from Nanoscale LiBH4 (Invited)

L. Shaw*, X. Wan, Y. Zhong, K. Crosby, University of Connecticut, United States

LiBH4 is one of the materials that have the highest gravimetric hydrogen density at room temperature known today. However, LiBH4 has been dehydrogenated and re-hydrogenated at high temperatures (e.g. > 400 C) because of its high chemical stability. In this study we report that nanoscale LiBH4 can release H2 at temperatures as low as 80 C with the peak releasing temperature at 165 C and the completion temperature at 275 C. These H2 release temperatures are the lowest ever reported in the open literature. Furthermore, no emission of borane, B2H6 – an impurity that is likely to poison polymer electrolyte membrane (PEM) fuel cells, is detected in the entire temperature range. Nanoscale LiBH4 can also alter the reaction pathway of the LiBH4+MgH2 mixture and reduce the hydrogen release temperature of MgH2 to ~150 C – the lowest temperature ever observed for MgH2. We believe that the unprecedented enhancement in the dehydriding behavior of LiBH4 and its mixture with MgH2 is due to the formation of sub-nm and low-nm LiBH4 particles, which results in a drastically reduced diffusion distance and thus the increased reaction kinetics. Furthermore, the associated improvement in the thermodynamic properties is responsible for the unusually low hydrogen release temperatures.

9:40 AM

(ENERGY-084-2010) Environmentally benign palladium membrane reactor for hydrogen production (Invited)

Y. H. Ma*, Worcester Polytechnic Institute, United States

Developing technologies to economically produce hydrogen with CO2 at high pressure suitable for sequestration is important to hydrogen economy and to protect environment. Pd membrane reactors can satisfy both requirements and are suited for process intensification by combining reaction, product concentration and separation in a single unit operation, providing high energy efficiency and low capital costs. An integrated catalytic membrane reactor and separator for producing pure hydrogen require membranes with long-term chemical, thermal and mechanical stability at high temperatures and pressures and high fluxes and separation selectivity. Our unique patented technologies for producing composite ultra thin Pd membranes satisfy all these requirements. An overview of the basis of composite Pd and Pd/alloy membranes for hydrogen separations will be discussed. The concept for improving the long-term thermal stability of composite Pd and Pd/alloy porous metallic substrate membranes by the controlled in-situ oxidation of the substrate and bi-metal multi-layer (BMML) deposition to generate an intermetallic diffusion barrier layer and their scalability will be presented. Materials challenges such as uniformity of the alloy films and membrane durability will be discussed based on the results obtained from HTXRD and XPS. The permeance of the prepared membrane has exceeded the 2015 target set by the US DoE.

10:20 AM

(ENERGY-085-2010) Nano-materials for Hydrogen Storage (Invited)

P. Jena*, Virginia Commonwealth University, United States

In order for the host materials to have gravimetric density of about 10 wt%, they have to consist of elements lighter than Aluminum. Unfortunately, the bonding of hydrogen in these materials is either too strong or too weak. Ways must, therefore, be found to tune the hydrogen bond strength so that host materials composed of light elements can be used as effective hydrogen storage materials. This talk will discuss how the novel properties of materials at the nanoscale can improve the thermodynamics and kinetics of hydrogen. In particular, I will discuss how carbon based nanostructures such as nanotubes and fullerenes can not only be used as catalysts to improve hydrogen uptake and release in complex light metal hydrides such as alanates, borohydrides, and imides but also how they can be functionalized with metal and B and Ca atoms to adsorb hydrogen in a novel quasi-molecular form. I will also discuss the role of electric fields in hydrogen storage. These results, based upon density functional theory and quantum molecular dynamics, provide a fundamental understanding of the interaction of molecular hydrogen with hosts consisting of light elements. It is hoped that the understanding gained here can be useful in designing better materials for hydrogen storage.Results will be compared with available experimental data.

10:40 AM

(ENERGY-086-2010) Novel Carbon Nanostructures Composites for Hydrogen Storage

R. Zidan*, M. A. Wellons, J. Teprovich, Savannah River National Laboratory, United States

not available

11:00 AM

(ENERGY-087-2010) Metal-Assisted Hydrogen Uptake on Nanoporous Carbon Materials (Invited)

C. Contescu*, V. V. Bhat, N. C. Gallego, Oak Ridge National Laboratory, United States

Adsorptive storage of hydrogen at near-ambient temperatures is intensively researched for hydrogen-fueled vehicles. A possible route for enhancing the hydrogen capacity of microporous materials is based on the mechanism of hydrogen spillover induced by addition of small amounts of transition metals with catalytic activity for hydrogen reactions. Spillover is a cascade of processes that consists of chemisorptive dissociation of molecules on catalyst sites, surface diffusion of atoms to secondary sites, and storage, reaction, or desorption. At ambient temperatures and elevated pressure, activated carbon fibers adsorb small amounts of hydrogen by physorption in narrow nanopores. Addition of small amounts of Pd to these carbon fibers causes a 30 % increase in the hydrogen amounts adsorbed at room temperature and 20 bar. We used adsorption measurements, in-situ high-pressure X-ray diffraction, and inelastic neutron spectroscopy to understand the underlying mechanism of enhanced hydrogen uptake. These techniques helped identify two of the elementary steps of the spillover mechanism: release of H atoms from Pd hydride particles destabilized by contacts with the carbon substrate, and chemisorption of H atoms to unsaturated sites on the carbon support. Recombination to physisorbed hydrogen accounts for the reversible part of excess hydrogen uptake.

11:20 AM

(ENERGY-088-2010) Dynamics of hydrogen adsorption on graphene and silicene: Ab initio computer simulations (Invited)

A. Farajian*, Wright State University, United States

Graphene and silicene, single-layer sheets of carbon and silicon, respectively, are among the novel materials with promising potentials for renewable and clean energy applications. This study focuses on the hydrogen adsorption properties of these materials. Specifically, we use ab initio molecular dynamics computer simulations to investigate the dynamics of hydrogen adsorption on these surfaces. We calculate the free energy barriers at different temperatures, when a hydrogen molecule approaches the surface. The free energy landscapes allow us to estimate the adsorptions rates. We compare the adsorption characteristics of graphene and silicene, and assess the suitability of these materials for hydrogen storage.

11:40 AM

(ENERGY-089-2010) The potential role of Mg-based hydrides for the improvement of negatives electrodes for advanced batteries (Invited)

M. Latroche*, ICMPE UMR7182 CNRS, France

The storage of hydrogen for either stationary or mobile applications is becoming more and more important in view of the coming 'hydrogen-driven-economy'. Numerous intermetallic alloys can reversibly store hydrogen at low to ambient pressures following two different ways: via the gas phase or electrochemically. For about two decades, most commercial rechargeable Ni-MH batteries employ LaNi5-based alloys that exhibit excellent properties as negative electrodes. However, they exhibit low capacities (only 1.2 wt.% hydrogen). To improve their weight capacities, such LaNi5-type compounds can be alloyed with MgNi2-type phase leading to so-called superlattice alloys that are now used as electrodes. However, real breakthrough will not be achieved without getting rid of heavy rare earths elements. Therefore, the search for new metal hydrides has focused on Mg-rich alloys, since pure Mg has a very high reversible storage capacity (7.6 wt%). Extremely sluggish sorption kinetics prevents practical application of MgH2 as a storage medium but Mg-(Sc,Ti) alloys have recently proven to be viable reversible hydrogen storage media. They were shown to have extremely high reversible electrochemical storage capacities up to more than 5 wt%, with discharge kinetics far superior to those of pure MgH2.

Battery Technology

Energy Storage and Conversion II

Room: Sawgrass
Session Chair: Gene Kim, Cookson Electronics Assembly Materials Group

8:00 AM

(ENERGY-090-2010) High Energy Density Metal Oxide Anodes for Li-ion Batteries (Invited)

A. C. Dillon*, C. Ban, L. A. Riley, Z. Wu, D. T. Gillaspie, National Renewable Energy Laboratory, United States; L. Chen, Y. Yan, S. Lee, University of Colorado at Boulder, United States

Significant advances in energy density and rate capability for Li-ion electrode materials will be necessary for implementation in electric vehicles. By employing metal oxide nanostructures, it is possible to achieve Li-ion anodes that have significantly higher energy density than the state-of-the-art graphite technology. We have demonstrated that thin film MoO3 nanoparticle electrodes (~2 μm thick) have a stable capacity of ~630 mAh/g at C/2[1]. By fabricating more conventional electrodes (~35 μm) with a conductive additive and binder, an improved reversible capacity of ~1000 mAh/g is achieved.[2] More recently we have focused on iron oxide nanostructures, as iron is an inexpensive, abundant and non-toxic material. We have synthesized binder-free, high-rate capability thin electrodes (~3μm). The electrodes contain Fe3O4 nanorods as the active lithium storage material and carbon single-wall nanotubes (SWNTs) as conductive additive. The highest reversible capacity is obtained using 5 wt.% SWNTs, reaching 1000 mAh/g (~2000 mAh/cm3) at C rate, for over 100 cycles. Furthermore, the electrodes exhibit high-rate capability and stable capacities of 800 mAh/g at 5C and ~600 mAh/g at 10C. Scanning electron microscopy indicates that this high-rate capability is achieved because Fe3O4 nanorods are uniformly suspended in a conductive matrix of SWNTs. Raman spectroscopy is employed to understand how the SWNTs function as a flexible conductive additive. We expect that our method can be used to achieve other binder-free electrodes with similar high-rate capability.

8:40 AM

(ENERGY-091-2010) Electrochemical performance of metal oxide coated LiNi0.5Mn1.5O4 material

A. Abouimrane*, H. Wu, I. Belharouak, K. Amine, Argonne National Laboratory, United States

There has been tremendous interest in recent years in the development of new cathode materials for high-power devices. These materials should be, low-cost, and provide high- power and energy-density characteristics, combined with long cycle-life over a wide range of temperatures. The spinel cathode LiNi0.5Mn1.5O4 originally proposed by Amine et al. has been extensively studied in the recent decade. Charge proceeds in predominantly two steps around 4.7 V with a theoretical capacity of about 149 mAh.g-1. Due to its high working potential, the energy density of LiNi0.5Mn1.5O4 is 20% higher than the traditional cathode material LiCoO2. Thus, LiNi0.5Mn1.5O4 is a potential candidate of high-energy cathode materials, which might be used in electric vehicles in the future. However, cells comprising LiNi0.5Mn1.5O4 suffer seriously from parallel electrolyte decomposition and dissolution of Mn and Ni during cycling and storage, especially at elevated temperatures. Surface modification has proved effective in improving the electrochemical performance of cathode materials. The structure and electrochemistry of the metal oxide coated 5V material will be discussed. The detailed analysis of 55C cycling performance will give insight into how this type of compound can be further improved in the future for lithium batteries application.

9:00 AM

(ENERGY-092-2010) Lithium Accumulator Capacity Increase via Three-Dimensional Construction of Electrodes

J. Prochazka*, L. Kavan, M. Zukalova, JHI, Czech Republic

The thin-film lithium battery technology has made a significant progress in past five years and in many aspects it has reached the theoretical possibilities. While the thin-film battery is nearly optimized, this work shows how to further extend the capacity limits of lithium accumulators by an original construction of 3D electrodes.

9:20 AM

(ENERGY-093-2010) Structure and Electrochemistry of Li2MnSiO4 Cathode Material

I. Belharouak*, A. Abouimrane, K. Amine, Argonne National Laboratory, United States

The candidate cathode material Li2MnSiO4 for lithium-ions cells was synthesized by an all-acetate precursor sol/gel method under a reducing atmosphere at 600, 700, and 800oC. The material prepared at 700oC was a pure phase and had the structural order of Li3PO4 orthorhombic (S.G. Pmn21) phase. The temperature dependence of the molar magnetic susceptibility of Li2MnSiO4 was found to be consistent with an antiferromagnetic material, with a Néel temperature of 12 K. The calculated effective moment confirmed that the observed magnetic behavior involves Mn2+ ions in a high spin configuration in tetrahedral sites. Scanning electron microscopy of Li2MnSiO4 showed large aggregates (10 to 50 microns) composed of nanosized particles (100-200 nm). The as-prepared material was almost electrochemically inactive despite the presence of 15 wt.% carbon additive. The material was treated by carbon coating using cellulose carbon source precursor and particle size reduction using high-energy ball milling. In coin-cell tests, the carbon-coated and ball-milling materials yielded charge capacities of 190 and 172 mAh/g, respectively, under a current density of 10 mA/g. At present, the cationic mixing between Li+ and Mn2+ ions in their mutual crystallographic sites is the main impediment to the achievement of the full theoretical capacity of Li2MnSiO4 (333 mAh/g).

9:40 AM

(ENERGY-094-2010) CZTS Monograin Materials for Photovoltaics

E. Mellikov*, Tallinn University of Technology, Estonia; D. Meissner, Crystalsol OÜ, Estonia; M. Altosaar, J. Raudoja, K. Timmo, T. Varema, M. Kauk, J. Krustok, O. Volobujeva, M. Danilson, Tallinn University of Technology, Estonia; K. Muska, T. Badegruber, W. Ressler, K. Ernits, F. Lehner, Crystalsol OÜ, Estonia

In monograin solar cells powders replace wafers or thin films. This allows for cheaper and much more efficient materials production minimizing materials loss. The separation of materials formation from the module fabrication - allowing for all temperatures and purity precautions– is the very important advantage. Large area module fabrication proceeds without any high temperature steps in a continuous roll-to-roll process. No upscaling problems arise as in thin-film technologies since a homogenous powder leads to homogenous modules. Solar cells from CZTS=Cu2(ZnxSn2-x)(SySe1-y)4) monograin powders have Voc up to 660 mV, fill factors up to 70 % and Isc more than 25 mA/cm2. Temperature coefficient of CZTS was measured to be below 2 mV/°K. Changing the sulfur/selenium ratio allows the change the band gap of CZTS between 1.04 and 1.72 eV.

10:20 AM

(ENERGY-095-2010) Lithium Storage Characteristics in Nano Graphene Platelets–based Materials (Invited)

C. Strope, T. Pham, H. Huang*, Wright State University, United States

Nano Graphene Platelets (NGPs) are referred to as one-layered graphene up to a few layers (less than 10 layers) of graphene sheets with basal area in submicro-scale. Since the one atomic-thick layer graphene was experimentally isolated in 2004, a sequence of scientific discoveries has revealed its various astonishing properties among all the existing materials, including the highest intrinsic mechanical strength, highest thermal conductivity, high surface area , and high electronic mobility etc. One feasible route to harness graphene's outstanding properties for immediate applications in lithium ion batteries at low cost will be based on nano graphene platelets (NGPs), which can be mass-produced via thermal exfoliation from graphite. NGPs have exhibited similar exceptional thermal, electrical, mechanical, and adsorptive properties of graphene and carbon nanotube, distinguished from other carbon nanomaterials. In this work, lithium storage characteristics in NGP powders with different average thicknessness were investigated. The NGPs were produced by Angstron Materials, our industrial collaborator, via electrochemical intercalation combining with thermal shock exfoliation. AFM was used to acess the thickness and basal dimension of the NGP specimens. Lithium storage in NGPs were characterized electrochemically by using Li counter electrode and 1M LiPF6-EC/DEC. This lithium storage capacity reached values twice that of graphitic carbon particles, which are also higher than many pyrolyzed carbon fabricated with less dimension control. Similar large reversible Li storage in graphite oxide was reported by others recently. Li storage characteristics in NGP/M nanocomposites were still under investigation.

11:00 AM

(ENERGY-096-2010) In-situ Impedance Measurements of LiMn1.5Ni0.4Cr0.1O4 Cathode During Charge/Discharge Cycling

K. Asmar, R. Singhal, R. S. Katiyar, University of Puerto Rico, Rio Piedras, Puerto Rico; A. Sakla, H. Abernathy, A. Manivannan*, US DOE, National Energy Technology Laboratoty, United States

LiMn2O4, LiMn1.97Co0.03O4, LiMn1.5Ni0.5O4, and LiMn1.5Ni0.4Cr0.1O4 cathode materials have been synthesized using sol-gel method for application in high energy density Li ion rechargeable batteries. The respective half cells were tested using cyclic voltammetry and charge discharge cycling. In-situ Electrochemical impedance spectroscopic measurements were performed before and after each charge and discharge cycle, respectively. After several cycles, Cr and Ni doped batteries proved to have a greater electrochemical performance than LiMn2O4. SEI (solid electrolyte interface) formation in the cathode caused a slight increase in impedance in the half cell that followed a decrease in discharge capacity. The differences in impedance measurements observed in-situ during charging and discharging cycles will be presented.

11:20 AM

(ENERGY-097-2010) Optimization of LixNi0.25CoyMn0.75-yO2±θ (x=1.225-1.65, y=0, 0.15) for High Energy Battery Applications

H. Deng*, I. Belharouak, H. Wu, K. Amine, Argonne National Lboratory, United States

Despite the number of extensive studies dedicated to the electrochemical properties of Li1.5Ni0.25Mn0.75O2.5 (also written as Li1.2Ni0.2Mn0.6O2) as an advanced cathode material for high energy lithium ion batteries in transportation applications, there are still issues related to understanding the material's structure, physical characteristics, and electrochemical behavior relationships. In this work, we explored the structural, morphological and electrochemical properties of lithium nickel manganese oxides by combining the effect of cobalt doping, various lithium contents, and surface coating. LixNi0.25CoyMn0.75-yO2±θ (y=0, 0.15) compounds were synthesized by solid state reactions between the coprecipitated spherical Ni0.25Mn0.75CO3 and Li2CO3 at 900oC. It has been found that tuning the lithium concentration in the materials was responsible for achieving improved electrochemical performances. Surface coating using AlF3 was also found to stabilize the interface of the cathode and hence helped in achieving high rate capability and good cycle life.

11:40 AM

(ENERGY-098-2010) Rapid Synthesis of Electrode Materials (Li4Ti5O12 and LiFePO4) for Lithium Ion Batteries Through Microwave Enhanced Processing Techniques

K. Cherian*, M. Kirksey, Spheric Technologies Inc, United States; A. Kasik, M. Armenta, S. Dey, Arizona State University, United States

The role of new batteries and energy storage materials are key factors in the new energy economy; certain new ceramic phases and rapid methods for their synthesis are, in turn, key to more efficient and cost-effective (especially Li ion) batteries. Such key phases can be prepared more rapidly and effectively through microwave enhanced processing wherein direct microwave heating as well as indirect and anisothermal microwave heating effects could occur; separated E & H field processing configurations could also offer tremendous advantages in this regard. Two examples of electrode materials which have been confirmed to form rapidly through special microwave processing approaches are Li4Ti5O12 and LiFePO4. Lithium carbonate and titania were the major starting reactants for microwave enhanced synthesis of the former, while the major starting reactants for the latter included lithium carbonate, ammonium dihydrogen phosphate and iron(II) oxalate. XRD analyses have confirmed the formation of the required phases. Additional analytical techniques including SEM was employed to characterize the phases formed. This paper discusses some preliminary experiments, results and subsequent investigations focused on developing faster, cheaper and greener synthesis routes for Li ion battery electrode materials.

Biomass

Materials Compatibilty with Biofuels

Room: Dunes 1&2

Session Chair: Edgar Lara-Curzio, Oak Ridge National Laboratory

8:00 AM

(ENERGY-099-2010) Addressing the Materials Challenges in Converting Biomass to Energy

C. Powell*, J. Bennett, B. Morreale, National Energy Technology Laboratory, United States

Converting biomass to energy offers an intriguing opportunity to reduce CO2 levels in the atmosphere, while simultaneously producing a value-added product in the form of electricity and/or liquid fuels. Utilized in combination with coal as the feedstock in a combustion or gasification cycle, biomass can provide a carbon-neutral source of renewable energy, without concerns for seasonal variations in feedstock availability. Utilized alone, biomass crops such as algae can be thermocatalytically converted to drop-in replacement fuels, while simultaneously storing CO2 emitted from point sources such as power plants. However, utilization of biomass-based feedstocks frequently results in an increase in the severity of the process environment, requiring the discovery and development of improved performance materials in order to make such processes economically viable. This talk will provide an overview of the on-going research at the National Energy Technology Laboratory to address the materials challenges in converting biomass and biomass-coal blends to electricity and liquid fuels via gasification and/or thermocatalytic conversion processes. Emphasis will be on the structural materials used in the construction of energy conversion systems, as well as the catalysts used to produce the final products.

8:20 AM

(ENERGY-100-2010) An Aggregation of Materials Composition Studies for Fuel Ethanol (Invited)

K. Moore*, Renewable Fuels Association, United States

The Energy Independence and Security Act of December 19, 2007 promotes environmentally sound transportation fuels and hopes to wean American consumers off of fossil fuels. This legislation promotes fuels from renewable, domestic sources and assures development of new fuels. Increased amounts of ethanol are expected. Transitioning new fuels affects every aspect of the fuel production, distribution and use chain. Wide variability exists in the test methods, fuel composition, and evaluation of impact and interaction of the material compatibility information. Existing transportation fuel handing equipment, such as tanks, piping, meters, safety devices, gaskets, etc., must be evaluated for suitability and exposure to new fuel compositions. Denatured fuel ethanol differs chemically from traditional petroleum derived transportation fuels. This abstract hopes to provide a review of denatured fuel ethanol characteristics and a historical perspective of materials compatibility testing completed to date. An additional component of the Energy Independence and Security Act promotes the use of nontraditional energy feed stocks. A discussion on the expected impacts of expanding past starch based ethanol production feed stocks will also be included.

8:40 AM

(ENERGY-101-2010) Overview of Materials Compatibility Issues with Fuel Grade Ethanol (Invited)

J. Beavers*, F. Gui, DNV Columbus, Inc., United States; A. Ertekin, N. Sridhar, DNV Research and Innovation, United States

There is significant interest within the North American pipeline industry in transporting fuel grade ethanol (FGE) as a result of the increased usage of ethanol as an oxygenating agent for gasoline and interest in ethanol as an alternative fuel. Currently, FGE is transported primarily by railroad tanker cars, tanker trucks, and barges. Several materials compatibility issues must be resolved before FGE can be transported in pipelines. These issues include stress corrosion cracking (SCC), corrosion, elastomer compatibility, and monitoring. For example, SCC has been observed in carbon steels in contact with FGE in user terminals, storage tanks, and loading/unloading racks. The Pipeline Research Council International (PRCI), the US Department of Transportation, Pipeline and Hazardous Materials Safety Administration (PHMSA) and individual pipeline companies have funded research to address these technical issues. This paper summarizes the results of recent research and the overall roadmap for future research to resolve the technical issues with transportation of FGE in pipelines.

9:00 AM

(ENERGY-102-2010) Compatibility Assessment of Fuel Dispenser Metals and Elastomers in an Aggressive E20 Fuel

M. Kass, S. Pawel, C. Janke, T. Theiss, S. Lewis, Oak Ridge National Lab, United States; W. Clark, National Renewable Energy Laboratory, United States; J. Chapin*, K. Boyce, T. Fabian, J. Bablo, Underwriters Laboratories, Inc., United States

Current energy needs are pushing to raise the ethanol content of gasoline from E10 (nominally, 10 vol.% ethanol) to levels approaching 20 vol.% (nominally, E20). The increase in ethanol concentration may cause compatibility issues with metal and elastomer components used in standard fuel dispensing equipment, which were originally designed for neat gasoline (minimal or no oxygenates). In this study a series of metal and fluoroelastomer coupons were exposed to an aggressive formulation of E20 known as CE20a per SAE J1681 standard. CE20a is a laboratory test fuel composed of 50 vol.% isooctane and 50 vol.% toluene (Fuel C)with 20% ethanol and aggressive additives (water, sodium chloride, acetic and sulfuric acid). The coupons were mounted in specially-designed sealed chambers that enabled a dynamic flow of the fluid at a constant temperature of 60oC. A portion of the samples were withdrawn after 4, 12 and 16 weeks of exposure. The metal coupons were analyzed for mass loss (corrosion) while the elastomer specimens were subjected to tensile strength and hardness measurements. The volume increase for the elastomers was also recorded. The results indicated that the mass loss for the metal coupons was low, but the surfaces of the brass, bronze and Terne steel coupons were highly discolored, which indicates that some level of surface oxidation had taken place. All of the elastomer properties were degraded to a higher degree in CE20a than in Fuel C. Standard nitrile rubber was used for comparison and suffered the highest property degradation of the elastomers tested. A number of high performance fluoroelastomers were evaluated in this study and several (Viton(tm) AC401, Dyneon(tm) FE5620, and Viton(tm) B601) exhibited increased swelling. Of the fluoroelastomers evaluated, Dyneon(tm) LFTE6400 and Viton(tm) GF-600S demonstrated the best combination of mechanical properties and low volume swell. The results indicate that property degradation is rapid (within 4 weeks of exposure) and that extended levels of exposure are unnecessary for coupon analysis.

9:20 AM

(ENERGY-103-2010) Microturbines and Biomass Fuels – Materials Challenges

W. Matthews*, Capstone Turbine Corporation, United States; K. More, L. Walker, Oak Ridge National Laboratory, United States

Anaerobic digester treatment of wastewater, agricultural waste and food processing waste produces methane and other gases. The biodegradation of waste material buried in landfills also produces methane and other gases. Traditionally, these sites have flared the waste gases, or vented them directly into the atmosphere. The "Capstone Renewable" MicroTurbines have been specifically designed to operate on these biomass fuels to provide renewable energy. While these biomass fuels contain useable energy, they also contain a number of contaminants such as hydrogen sulfide (H2S), and siloxanes, along with various other contaminants. The Capstone CR30 is capable of operating on biomass fuels with H 2S levels as high as 7% (70,000 ppm), while the CR65, CR200 and CR1000 family are capable of operating on biomass fuels with H2S levels up to 0.5% (5,000 ppm). The Capstone liquid fuel MicroTurbines also operate on bio-diesel. While bio-diesel has low sulfur content it does tend to contain other contaminants, such as Sodium and Potassium, which can be very detrimental to the hot section components of the MicroTurbine. The materials challenge is to develop hot section materials solutions that are more resistant to sulfidation and hot corrosion in the presence of high levels of H2S and sulfur, and other contaminants such as Sodium and Potassium.

9:40 AM

(ENERGY-104-2010) Material Characterization and Analysis for Selection of Refractories Used In Black Liquor Gasification

J. G. Hemrick*, J. R. Keiser, R. A. Peascoe-Meisner, Oak Ridge National Laboratory, United States

Black liquor gasification provides the pulp and paper industry with a technology which could potentially replace recovery boilers with equipment that could reduce emissions and, if used in a combined cycle system, increase the power production of the mill allowing it to be a net exporter of electrical power. In addition, rather than burning the syngas produced in a gasifier, this syngas could be used to produce higher value chemicals or fuels. However, problems with structural materials, and particularly the refractory lining of the reactor vessel, have caused implementation of this technology to be problematic due to unplanned shutdowns replacement of components much sooner than originally planned. Through examination of exposed materials, laboratory corrosion tests and cooperative efforts with refractory manufacturers, many refractory materials issues in high-temperature black liquor gasification have been addressed and optimized materials have been selected for this application. In this paper, the characterization and analysis techniques used for refractory screening and selection will be discussed along with characteristic results from these methods which have led to the selection of optimized materials for this application.

10:20 AM

(ENERGY-105-2010) Performance of Materials in Biomass Gasification systems

J. R. Keiser*, P. J. Blau, B. A. Pint, Oak Ridge National Laboratory, United States; R. A. Meisner, University of Tennessee-Knoxville, United States; J. G. Hemrick, Oak Ridge National Laboratory, United States

The thermochemical route for utilization of biomass resources is a very efficient path to produce syngas or a liquid product. However, experience gained during operation of demonstration and commercial scale gasification systems has shown that the environments produced in many of these systems are very aggressive toward the materials used in the containment structures. To better understand the degradation mechanisms, damaged components have been examined and laboratory simulation studies involving both corrosion and wear have been conducted allowing the identification of alternate materials. While these alternate materials have successfully addressed many of the problems encountered, many proposed gasification systems call for higher temperatures and even more severe environments. It is expected that these increased demands on structural materials will require additional evaluations and new materials solutions.

10:40 AM

(ENERGY-106-2010) Volatility of Inorganics During the Gasification of Dried Sludge

C. Bourgel*, J. Poirier, CNRS-CEMHTI, France; F. Defoort, J. Seiler, CEA/DTN/SE2T/LTE, France; C. Peregrina, Material recycling and energy recovery Division, CIRSEE, France

The context of the present study relates to the gasification of dried sludge under high temperature. The aim of this work is to shed new light on the impacts of sludge ashes in gasification process. The purification sludge can contain more than 50% of inorganic matter. The objective of this study is to understand the role of these inorganics during the heating. Several techniques are used to solve this problem. First, using thermodynamic calculations (Factsage®) the evolution of the volatility of the inorganics is observed and the condensed phases formed during the heat treatment are determined. The simulations are done under atmospheric pressure condition, from 500 to 1500°C. Second, to compare with the calculus, an XRD and XRF in situ measurement experiment is developed in the CEMHTI Laboratory in order to determine which species volatilize. The major elements of the sludges are Si, Al, Fe, P and Ca. The calculations allow us to determine the formed gases, and the condensed phases during heat treatment. The major formed gases are CO, H2, H2O, CO2, CH4 and N2. The minor formed gases are H2S, COS, HF, HCl and NH3. On the contrary, the Na, K, Fe and P elements don't volatilize entirely during the heating. Indeed, they are found in the condensed phases formed of sodium and potassium alumino-silicate, iron silicate and calcium phosphate. Finaly, these results will be confronted to the experimental measurements.

11:00 AM

(ENERGY-107-2010) Catalysts and Sorbents for Thermochemical Conversion of Biomass—Material Development Needs

S. Cheah*, K. Magrini-Bair, National Renewable Energy Laboratory, United States

Rising world demands for oil and a finite petroleum reserve have increased interest in alternate liquid fuel sources that are diverse, secure, and affordable. Biomass is a renewable source of carbon that is abundant in many regions of the world. The focus of next generation biofuels is to produce fuel derived from cellulosic biomass. Thermochemical conversion of biomass to fuels is a viable route that has the potential to be cost competitive with gasoline, as well as biochemical biomass conversion processes. Several different routes of thermochemical conversion, including production of bio-oil through pyrolysis and subsequent bio-oil upgrading; production of syngas through gasification of biomass, and subsequent fuel synthesis from syngas will be discussed. The material development needs in each stage will be identified. For example, to efficiently transform biomass into bio-oil via pyrolysis or syngas via gasification, next generation catalysts for catalytic pyrolysis and catalytic gasification are necessary. New developments in high temperature clean-up of syngas will improve thermal efficiency and process economics of biomass conversion. The bio-oil that is produced from pyrolysis has high oxygen content, and challenges in the development of hydrodeoxygenation catalyst shall be discussed.

11:20 AM

(ENERGY-108-2010) Air Force Research Lab Bio Technology (Invited)

O. Mendoza*, Air Force Research Lab, United States

CO2 absorption along with bio-fuels are military priorities. The Air Force Research Laboratory has large scale algae reactors and leads the way to bio-energy for the military. The work performed is crutial for designing the bio-fuel blue print that the military would need from industry to build a sustainable energy source. Technology advances that have made the AF a leader will be presented.

11:40 AM

(ENERGY-109-2010) Solid Catalysts from Biochar

J. Kastner*, D. Geller, J. Miller, University of Georgia, United States; L. Keith, Down to Earth Energy, LLC, United States

Recently there has been renewed interest in the synthesis of solid acid and base catalysts, primarily driven by the need to find "green" catalysts to replace waste generating homogeneous acids and bases. Our research group has successfully synthesized solid acid and base catalysts from peanut hull and pine biochar. Catalysts were generated by pyrolyzing biomass at low temperatures to generate a carbon backbone. Next, the carbonized materials were sulfonated and subsequently washed and dried. The sulfonated biochars were subsequently tested for their ability to esterify free fatty acids with methanol. Esterification of the fatty acids was typically complete (90-100% conversion) within 30-60 minutes at 55-60C. Drying of the char based acid catalysts for 1 hour at 125C between uses maintained esterification activity, thus allowing the catalysts to be reused. Solid base catalysts were also synthesized from biochar by attaching ethylenediamine and 4-aminophenoxide to the surface. One base catalyst generated from peanut hull char was shown to completely convert soybean oil within 3 hours at 65C, comparing favorably to the commercial sodium methoxide catalyst. Building on this success, we have recently demonstrated that the solid acid catalysts synthesized from peanut hull or pine chip char are capable of hydrolyzing cellobiose and xylan to glucose or xylose.

Wind

Materials Trends and Opportunities for Wind Energy Applications

Room: Sea Oats
Session Chairs: Tom Ashwill, Sandia; Douglas Cairns, Montana State University

8:00 AM

(ENERGY-110-2010) Selection of Wind Turbine Blade Materials for Fatigue Resistance

J. F. Mandell*, Montana State University, United States

Wind turbine blades are subjected to severe fatigue loading over their 20-yr. or longer lifetime. The blade laminate constituents must be selected for fatigue resistance over a range of conditions including tension, reversed loading and compression. The paper will compare the relative performance of the major reinforcing fibers, fabric architectures and resin types based on a 20-yr. testing program. Interaction effects of infusion molding details (one-side vs. two-side tooling) and reinforcing fabric architecture will be discussed. Data will be presented for both standard (in-plane) laminate properties and interlaminar properties which are critical at structural details.

8:20 AM

(ENERGY-111-2010) Materials Solutions for Wind Energy (Invited)

P. J. Dougherty*, SMI Inc./Helios Strategies, United States

Although wind technology currently provides only 1% of the U.S. electric power needs, the U.S. wind industry continues to expand at over 25% annually, with over 31,000 megawatts of generation installed in the U.S. as of mid 2009. Utility-scale generators, approaching between 300 and 400 feet from tower base to blade tip, are operating in 37 states. However, wind energy faces a number of siting concerns across jurisdictions, including potential impacts to wildlife, visual impact, and interference with military and civilian radar as well as microwave signals. The use of advanced designs and materials in wind blades offers a solution to mitigate these interactions at low cost, thus maintaining the financial viability of a wind project.

8:40 AM

(ENERGY-112-2010) Advanced Composite Materials and Manufacturing Processes Increase Wind Turbine Size and Reliability

M. Tupper*, M. Hulse, J. Cronin, W. Francis, K. Mallick, CTD, United States

The size of wind turbines has grown driven by a desire for increased energy capture. Land-based wind turbines have increased from 50kW to 3 MW driven primarily by increased blade length. Further increasing blade length represents a significant challenge. To achieve, this materials with increased stiffness to minimize deflections during operation, lower density to minimize blade mass, and higher fatigue strength to reduce material degradation thereby maximizing blade life are required. Furthermore, the reliability of composite wind turbine blades is principally dependent on manufacturing quality, which can significantly impact the blades fatigue performance. Issues impacting blade reliability include manufacturing defects within the composite laminates, de-bonding of adhesive joints, and degradation of the resin due to microcracking and the environment. A combination of advanced materials, including microcrack resistant resins, localized improvement of adhesive shear properties using nano reinforcements, and advanced tooling based on shape memory foam allowing for more efficient structural designs can provide higher operating margins for blade structures.

9:00 AM

(ENERGY-113-2010) Materials Challenges and Opportunities in Wind Energy (Invited)

F. D. Marquis*, Naval Postgraduate School, United States

The Wind power available on the Earth atmosphere is much larger then the current world power consumption. Its potential on land and near shore is believe to exceed 72 TW. This is equivalent to 54 millions of tons of oil per year, or over five times the total combined world power from all sources. In addition wind power is clean and renewable without any form of emissions or residues and it does not involve the depletion of any form of fuel. The growth in new capacity has exceeded 30 percent over the last five years and is expected to continue and/or exceed this trend for many years to come. This means that the wind power industry is currently experiencing a very rapid development stage but is far from reaching its mature stage. Currently it faces many important challenges and opportunities but its potential is extraordinary. The environmental impacts are very few but not in depth such as noise and potential disturbance in landscape, fauna and flora. Advances in power grid characteristics and recharging technology are expected to be considerable enablers. This paper discusses typical challenges and opportunities in mechanical and materials design and manufacture with particular focus on the potential of nano-composites and hybrid materials for application in new environments and geographic locations both land-based and offshore.

9:20 AM

(ENERGY-114-2010) Effects of Fiber/Matrix ratios and Dry and Wet Environments on the Mechanical Properties of Carbon/Polyurethane Composites

M. Farooq*, C. Lazzara, J. Bicerano, P. Viens, Neptune Research Inc., United States

Carbon/polyurethane composites could be potentially viable directly and/or repair in marine and alternative renewable energy applications. Carbon/polyurethane composites are made with different fiber volume fractions and tested in 0° and 90° orientations. Prepared specimens were immersed in distilled water and saltwater at room temperature and tested to determine water effects on the mechanical properties of carbon/polyurethane composites. 0° orientation and higher volume fraction showed higher tensile strength in dry conditions compared to 90° orientation.

10:00 AM

(ENERGY-115-2010) Embedded Sensors for Composite Wind Turbine Blades

D. Cairns*, Montana State University, United States

Background and Impetus Wind energy is rapidly being developed as an alternative energy generation technology. In this paper we discuss and quantify several aspects of the deployment of composite wind turbine blade sensors. We have explored several low cost sensors for embedment into composite wind turbine blades. The focus of this paper is on manufacturing studies with PVDF sensors, metal foil strain gages (MFSG), and Fiber Optic (FO) sensors for strain and load monitoring. Summary Conclusions The mechanical performance of wind turbine blade composite laminates with embedded sensors is highly dependent on the interface bonding between sensor and surrounding composite. Constitutive material properties have shown no appreciable change as a consequence of the embedded sensor. Despite the common idea that fiber optics would be a less disruptive sensor to integrate into composite materials, it is clear from testing that such a sensor must be surface treated as well to insure proper integration. Further improvements may require collaborations with the fiber optic manufacturers to improve the mechanical performance of this region. A hierarchical procedure for evaluating the mechanical performance of composite laminate was developed and discussed. This provides a basis for future work with the development and integration of new, low cost sensors for composite wind turbine blades.

10:20 AM

(ENERGY-116-2010) Printed Sensors for System State of Health Monitoring

P. Clem*, C. A. Apblett, E. D. Branson, J. F. Carroll, K. R. Fenton, Sandia National Laboratories, United States

As energy demand rises, the need for reliable electrical generation and distribution becomes more critical. Instrumenting existing generation and distribution systems to improve monitoring and reliability often requires placement of sensor networks into complex environments. The need for cheap, reliable, flexible, conformal sensors that can give diagnostic state of health information motivates the development of materials that can be printed onto the monitored system, or provide the needed flexibility of substrate to allow integration of sensors without shutting down the network or generator. In this talk, we present materials research in the direct printing of four basic types of sensor systems: printed thermocouples for close access temperature monitoring, printed strain gauges for mechanical and vibration monitoring, printed electrochemical arrays for monitoring corrosion, and printed antennas for monitoring near field RF emissions. Each sensor type places different demands both on the formulation of the ink, as well as the post processing of the inks into the materials for these sensor applications. Performance data from each type of sensor will be presented. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the US Department of Energy's NNSA under Contract DE-AC04-94AL85000. This work was supported by the Sandia National Laboratories LDRD program.

10:40 AM

(ENERGY-117-2010) Development of Multifunctional Nanocomposite Coatings for Wind Turbine Blades

J. Gou*, Y. Tang, F. Liang, J. Kapat, University of Central Florida, United States

The research and development of nanocomposite materials has gained significant attention in recent years due to their potential applications in the engineering, medical, and defense fields. We recently explored a unique concept of manufacturing nanocomposite coatings with carbon nanotube/nanofiber/graphene based nanopapers for wind turbine blades. This approach involves making carbon nanopaper by the filtration of well-dispersed carbon nanotubes/nanofibers/graphene under controlled processing conditions. The carbon nanopaper has excellent mechanical, electrical, and thermal transport properties. In our research, carbon nanopapers are integrated into fiber reinforced composite laminates using liquid composite molding processes such as Vacuum Assisted Resin Transfer Molding (VARTM). Several applications of carbon nanopaper based nanocomposite coatings for wind turbine blades are illustrated; in particular, structural and acoustic damping, lightning strike protection, and sand blasting mitigation.

11:00 AM

(ENERGY-118-2010) Novel cost-effective materials and processes for Wind Energy

A. Kumar*, Z. Liang, B. Wang, C. Zhang, O. Okoli, T. Liu, C. Zeng, A. Vanli, M. Zhang, HPMI, Florida State University, United States

The High-Performance Materials Institute (HPMI) at Florida State University (FSU) is developing novel cost-effective composite and nanomaterial technologies that can be directly used by the wind energy community. These include (1) Resin Infusion between Double Flexible Tooling (RIDFT), which is capable of rapidly and inexpensively producing composite parts in mass or for individual specifications for various applications, (2) High-temperature resin transferring molding and vacuum-assisted resin transferring molding (RTM/VARTM), which produces high quality composites parts, (3) Nanomaterial technology to incorporate multifunctional properties and processes to develop sheets of nanomaterials called buckypapers for ease of use and integration into wind energy components. This presentation will focus on these technologies and their potential applications to wind energy. Details and preliminary results on the use of the materials and processes for applications such as fire retardancy, lightning strike protection, multifunctional nanofoam, rapid prototyping, EMI shielding etc. will also be presented.

11:20 AM

(ENERGY-119-2010) Nanostrength® Block Copolymers for Wind Energy

R. Barsotti*, J. Chen, A. Alu, Arkema, Inc, United States

One of the current challenges in the widespread adoption of wind energy is the ability to make larger, more reliable wind blades without significantly increasing the weight of the blades. Increase in service life is needed for both wind blade composites and adhesives. Thermoset composites and adhesives are valued for excellent strength, chemical resistance and high temperature properties but suffer from low toughness. For wind energy applications, it is necessary to improve the fracture toughness and fatigue performance of blades and adhesives without effecting mechanical properties such as strength or modulus or processing variable such as viscosity or curing kinetics. Although many additives exist for improving the toughness of thermosets exist, most are difficult to incorporate into formulations or result in a "trade-off" of properties. Arkema's controlled radical polymerization technology has been used to synthesize Nanostrength® block copolymers additives, which provide excellent toughening to thermosets at low loading levels without sacrificing other properties. By incorporating functionality into the thermoset miscible block of the polymer, different nano-morphologies of these polymer additives are achieved in a wide range of thermoset systems. By controlling structuration of these polymers, a wide range of mechanical properties can be achieved.

Hydrogen

Characterization and Analysis of Hydrogen Storage Materials

Room: Seashore Ballroom
Session Chairs: Ashley Stowe, B&W Y-12 National Security Enterprise; Sonjong Hwang, Californina Institute of Technology

1:40 PM

(ENERGY-120-2010) Characterization Studies of Boron-Containing Compounds for Hydrogen Storage Applications (Invited)

R. C. Bowman*, Oak Ridge National Laboratory, United States; S. Hwang, C. Kim, California Institute of Technology, United States; G. M. Brown, D. A. Knight, Oak Ridge National Laboratory, United States; J. Zhao, The Ohio State University, United States; J. W. Reiter, J. A. Zan, Jet Propulsion Laboratory, United States; G. L. Soloveichik, S. Kniajanski, GE Global Research, United States

Several light metal borohydrides, ammine borohydride complexes, and aluminoboranes have been prepared and investigated as potential hydrogen storage candidates. The storage capacities and desorption properties have been measured by volumetric methods while phase compositions and reaction products were characterized by solid-state nuclear magnetic resonance and x-ray diffraction. All of these hydrides were found to release over 10 wt% hydrogen upon heating to elevated temperature along with generating amorphous decomposition products that can include dodecaboranes, metal borides, and boron nitride species depending upon compositions and desorption conditions. The presence of the more highly stable intermediate or final phases inhibits regeneration of the original compounds that severely impact their performance for reversible hydrogen storage applications. Possible reaction mechanisms will be presented and discussed.

2:00 PM

(ENERGY-121-2010) Multinuclear High Resolution Solid State NMR studies of Dodecaborate Intermediate of Borohydrides based Hydrogen Storage Systems

S. Hwang*, C. Ahn, J. W. Reiter, J. A. Zan, California Institute of Technology, United States; V. Stavila, Sandia National Laboratories, United States; J. J. Vajo, HRL Laboratories, LLC, United States

Formation of boron clustered reaction intermediates such as metal dodecaborane, M[B12H12]x (M=Li, Mg, Ca), has been a central issue in investigation of complex metal borohydrides materials for hydrogen storage applications. We have performed thorough studies on this issue in two aspects: 1) change in reaction pathway and minimization of the intermediate formation, 2) reactivity of metal dodecaborane in various reaction conditions. Multinuclear (1H, 11B, 6,7Li) Magic Angle Spinning (MAS) NMR, cross Polarization (CP) MAS, and multiple quantum (MQ) MAS NMR methods as well as other spectroscopic tools were employed to carry out characterization of structural changes and phase identification. Application of hydrogen back pressure during the dehydrogenation process was identified as a key reaction condition to bypass the dodecaborate formation certain cases, such as in LiBH4+MgH2 system. In the reactivity search of MnB12H12 or MnB12H12 + (12/m)MHm, nearly no reaction was observed probably due to a kinetic barrier. Use of some extreme treatment will be discussed as a method of boosting some reactivity.

2:20 PM

(ENERGY-122-2010) Contributions from anelastic spectroscopy to the study of complex hydrides (Invited)

R. Cantelli*, Sapienza University of Rome, Italy; A. Paolone, CNR-INFM Laboratorio Regionale Supermat, Italy; O. Palumbo, ISC-CNR Istituto dei Sistemi Complessi, Italy; P. Rispoli, Sapienza University of Rome, Italy

Recent results obtained by anelastic spectroscopy in complex hydrides are presented. The information provided is often highly requested in the studies of novel materials for hydrogen storage. It supplies the local and long-range dynamics of hydrogen and other mobile entities, the phase transformations and the time and temperature resolved evolution of the hydrogenation/dehydrogenation reactions. Experiments on undoped and Ti-doped NaAlH4 first revealed the formation, during decomposition accompanying the dehydrogenation reactions, of a highly mobile species containing hydrogen, which is likely constituted by a vacancy complex of type AlH6-x. The obtained data allowed the proposition of a model for the dehydrogenation process, which assigns to Ti a trapping action on hydrogen which lowers its dissociation energy in the bond and makes the decomposition reversible. In ammoniaborane, NH3BH3, a thermally activated relaxation peak is observed around 100 K (at 1 kHz) which we attributed to the torsional and rotational motions of the NH3 and BH3 ends. A systematic study of the structural transition occurring around 220 K in NH3BH3 and in its isotope substitutions was performed. It was also shown that the dispersion of NH3BH3 as a single monolayer inside silica scaffolds suppresses the phase transformation, proving that nanoconfining modifies the properties of NH3BH3.

2:40 PM

(ENERGY-123-2010) New Possibilities for Understanding Complex Metal Hydrides via Synchrotron X-ray Studies

T. A. Dobbins*, Louisiana Tech University, United States

This research seeks to understand the role of catalysts in hydride structures. X-ray absorption spectroscopy is used to examine the chemical interaction of catalysts (TiCl3) with the host hydride powder (NaAlH4). Results show that TiCl3 transforms first to metallic Ti—then reacts with Al3+ in NaAlH4 to form TiAlx complexes. It remains unclear, however, whether the formation of those TiAlx complexes is directly related to catalysis of the H2 desorption reaction in the hydride. Ultrasmall angle x-ray scattering (USAXS) is used to study trends in powder surface area with various treatments. Powder surface area is an indicator of hydride particle damage accumulation (i.e. crack formation in and fracture of the particle) during high energy ball milling to add catalysts and during hydrogen desorption. Sodium alanate (NaAlH4) powders are routinely high energy milled with the transition metal salt catalysts, TiCl2, TiCl3, ZrCl4, and VCl3. Results show that NaAlH4 has an inherently high surface area (characterized by the surface fractal morphology) and that after catalyst introduction by high energy ball milling, higher surface areas are retained for catalysts which show the best desorption kinetics and lowest surface areas are yielded for poorly performing catalysts. After desorption, the surface area was lower, relative to the undesorbed powders, in all cases.

3:00 PM

(ENERGY-124-2010) Structural study and hydrogen sorption kinetics of ball-milled samples of cast Mg-10%Ni catalysed by Nb

S. Aminorroaya-Yamini*, A. Ranjbar, H. K. Liu, University of Wollongong, Australia; Y. Cho, A. K. Dahle, University of Queensland, Australia

It is known that Mg2Ni facilitates the hydrogen molecules dissociation in the composite Mg-Mg2Ni and enhances hydrogen diffusion at phase boundaries. To further improve the hydrogen sorption kinetics, Nb has been introduced to Mg-Mg2Ni composite. In the present study, the eutectic structure of cast Mg-10wt%Ni was refined by addition of 1wt% Nb into the melt during casting. The chips of cast Mg-10%Ni and Mg-10%Ni-1%Nb ball-milled separately and then with 5wt% MW-CNTs and 5wt% Nb. SEM analysis was carried out on cast and ball-milled samples to study the microstructure and distribution of Nb and Mg2Ni. The absorption and desorption kinetics of samples were measured at 350, 250, 200 and 100°C by Sieverts's method apparatus. The results showed that 1%Nb addition during casting accelerates the hydrogen diffusion compare to cast Mg-10%Ni. However, addition of 5% MW-CNT to ball-milled powders showed no effect on kinetics of absorption/desorption while improved the activation characteristics of the samples significantly. It might occur due to reaction with oxide layers during activation procedure. The absorption/desorption kinetics in addition to hydrogen capacity of the sample contained 5% Nb improved considerably even at temperatures as low as 100°C. TGA/DSC results showed that the releasing temperature decreased by 30-50°C compare to ball-milled Mg-10%Ni sample.

3:40 PM

(ENERGY-125-2010) Recent Results from DOE's Chemical Hydrogen Storage Center of Excellence (Invited)

K. Ott*, Los Alamos National Lab, United States

Hydrogen as a liquid or a compressed gas has a high gravimetric energy density, but a very low volumetric energy density which restricts the range of hydrogen vehicles. Storing hydrogen in compounds is one approach to providing higher volumetric densities of hydrogen. Chemical hydrogen storage involves release of hydrogen from compounds containing strong covalent chemical bonds using various pathways such as hydrolysis, thermolysis, or catalysis. Recent results from DOE's Chemical Hydrogen Storage Center of Excellence will be presented. This Center's work focuses on developing energy- and cost-efficient processes that release hydrogen from covalent amine borane compounds, and the efficient chemical regeneration of the spent fuels. Much of the Center's work is directed at releasing hydrogen from amine-borane compounds such as ammonia borane and the related metal-substituted derivatives. I will discuss the various thermal and catalytic options for releasing hydrogen from these compounds, recent results in the off-board chemical regeneration of the spent fuel, and preliminary cost estimates of several of these options related to using ammonia borane as a storage material. Last, near term opportunities for stationary, portable and other niche vehicular applications of chemical hydrogen storage will be discussed.

4:00 PM

(ENERGY-126-2010) In-situ neutron diffraction for characterization of hydrogen storage and infrastructure materials (Invited)

L. Laversenne*, L. Cagnon, P. De Rango, D. Fruchart, CNRS Institut Neel, France; J. Huot, IRH-Universite du Quebec a Trois-Rivieres, Canada; S. Miraglia, V. Nassif, CNRS Institut Neel, France; S. F. Santos, IRH-Universite du Quebec a Trois-Rivieres, Canada; N. Skryabina, Perm State University, Russian Federation

The relevance of in-situ neutron diffraction experiments for investigation of materials related to hydrogen energy will be presented . Dynamical studies of hydrogen absorption and desorption performed through the implementation of solid-gas reaction and electrochemical charging/discharging will be described. Experiments have been performed at Institut Laue Langevin (ILL Grenoble, France) using D20, D1B and D1A high resolution diffractometers. Neutron diffraction is complementary to X-ray diffraction since it presents the advantage that light atoms (deuterium) contribute strongly to the diffracted intensity. This experimental work leads to a better understanding of fundamental mechanisms of hydrogen insertion in materials. In the context of search for effective materials for solid hydrogen storage, we will present the study of structural evolution in intermetallic bcc compounds during hydrogenation-dehydrogenation. Moreover, investigation of hydrogenation mechanism in activated magnesium will be described. Concerning infrastructure materials, a study of hydrogen embrittlement in iron based alloy with sigma phase will be presented.

4:20 PM

(ENERGY-127-2010) Analysis of Cryosorption System for Hydrogen Storage (Invited)

R. Chahine*, HRI - Universite du Quebec a Trois-Rivieres, Canada

Significant R&D efforts are being pursued globally to improve the efficiency and economics of onboard hydrogen storage systems for mobile applications. The sorption of hydrogen on or in a solid substrate, relying either on physisorption or chemisorption or even a combination of both offers a potential alternative means of storing hydrogen. Hydrogen storage via physisorption on porous materials, such as activated carbon, carbon nanostructures and metal organic frameworks (MOFs) is particularly enticing due to its inherent reversibility and cyclability. Moreover, these materials exhibit fast kinetics and operate at relatively low storage pressures. However, hydrogen physisorption at ambient temperatures on currently available porous materials leads to unacceptably low hydrogen storage densities. Acceptable densities are only attainable at cryogenic temperatures. We will present the results of our evaluation of an adsorption-based hydrogen storage tank for vehicular application. We will discuss the net storage capacity of the system over wide temperature and pressure ranges, the thermal requirements to charge and discharge hydrogen at the desired flow rates, and dormancy.

4:40 PM

(ENERGY-128-2010) Analysis of Thermal Decomposition of t-Butylamine Borane (Invited)

A. C. Stowe*, N. Smyrl, J. Morrell, J. Feigerle, B&W Y-12 National Security Enterprise, United States

Amine boranes are a class of materials which release significant yields of hydrogen gas upon heating to temperatures relevant for automotive applications. The thermodynamic stability of this class of amine boranes is correlated with the extensive di-hydrogen bonding between boron hydrides and amine protons. Further, the hydrogen evolution follows a bimolecular pathway via the di-hydrogen bonding network. The thermal decomposition of t-butylamine borane (tBuAB), $(CH_3)_3CH_2NBH_3$, has been studied in order to understand the reaction pathway of hydrogen sorption and the impact of the t-butyl substitution dehydrogenation thermodynamics. ^1H, ^{11}B, and ^{13}C solid state nuclear magnetic resonance (NMR) spectroscopy has revealed that heating initiates two separate reaction pathways: isomerization and hydrocarbon abstraction resulting in varying yields of isobutane and hydrogen. It is also possible that tBuAB dissociates about the N-B bond giving rise to borane stretching modes in the gas FTIR. ^{11}B NMR indicates that the major reaction pathway results in hydrogen evolution with isobutane formation being present in smaller yields. The t-butyl substitution lowers the thermodynamic stability—compared to NH_3BH_3—but results in impure hydrogen gas stream and lowered capacity due to isobutene evolution.

Battery Technology

Energy Storage and Conversion III

Room: Sawgrass
Session Chairs: Vijay Jain, URS Washington Division; Joshua Gray, Savannah River National Laboratory

1:40 PM

(ENERGY-129-2010) HeteroFoaMs: A New Frontier in Energy Storage and Conversion Materials

K. Reifsnider*, F. Rabbi, Univ. of South Carolina, United States

Heterogeneous Functional Materials (HeteroFoaMs) are a unique class of materials in which the nano-structure (composition, arrangement, morphology, and connectivity) literally controls the functional performance at the global level. Multi-physics modeling, and even property determination at the nano-level is a fundamental challenge in the conception and design of such heterogeneous materials. A DoE Energy Frontiers Research Center has been formed by seven universities and two national labs to address this challenge. The present paper will outline their approach and report some early findings of that Center. Special attention will be given to the problem of defining properties and behavior for heterogeneous nano-phased materials on a scale that controls functional performance of solid oxide fuel cell electrodes. Demonstration of concepts will be attempted with the help of analysis and experimental data for voided heterogeneous materials under the excitation of alternating current fields. Initial observations and future directions will be presented.

2:00 PM

(ENERGY-130-2010) Development of Nano/Micro-structured Materials for Energy Storage (Invited)

H. Cheng*, Chinese Academy of Sciences, China

Energy is one of the most important topics in the 21st century. With the rapid depletion of fossil fuels and increasingly worsened environmental pollution caused by vast fossil energy consumption, it is in a high demand to make efficient use of energy and to seek for renewable and clean energy sources. Research and development of new energy storage materials have received worldwide concern and increasing research interest The Institute of Metal Research has been working on energy materials in recent years, and its activities are briefly introduced. And then the research and development of energy storage will be reported. A hierarchical porous carbon with facilitated ion transfer rate and good electronic conductivity, hybrid energy storage device design, graphene/conductive polymer composites, graphene/oxide composites, and carbon nanotubes to modify conventional micrometer-sized electroactive materials are developed for supercapacitors and lithium ion batteries.

2:20 PM

(ENERGY-131-2010) Development of Advanced Low-Temperature Sodium-Beta Alumina Batteries

X. Lu*, G. Xia, K. Meinhardt, J. Lemmon, V. Sprenkle, Z. Yang, Pacific Northwest National Laboratory, United States

Due to the high round-trip efficiency and capability of energy storage for a duration of hours, the sodium-beta alumina battery technologies have gained increasing interests for renewable and utility applications. The batteries are typically fabricated upon a thick tubular β”-alumina electrolyte (> 2 mm) with a relatively high operating temperature (> 300°C) to achieve adequate cell performance. Recently, we attempt to develop battery cells constructed on a thinner planar electrolyte. At the meanwhile, research work has been conducted to modify the cathode both the microstructure and composition in such a way that a satisfactory performance can be achieved at a lower temperature. The details of the work the paper will be presented.

2:40 PM

(ENERGY-132-2010) Ionogels as Solid Electrolytes for Advanced Battery Applications

J. Gray*, H. Colon-Mercado, B. Garcia-Diaz, A. Visser, M. Williamson, M. Au, T. Adams, Savannah River National Laboratory, United States

This research investigated the use of solid-state supported ionic liquids (ionogels) as possible electrolyte phases for lithium ion battery applications. Techniques were developed to measure the conductivity of both ionic liquids and ionogels using galvanostic step and electrochemical impedance spectroscopy techniques. The conductivities of several ionic liquids were found to be between 10^{-6}-10^{-3} S/cm. One of the ionic liquids that successfully formed a lithiated iongel possessed a conductivity an order of magnitude greater than the constituent ionic liquid (10^{-3} vs 10^{-4} S/cm), which was on the order of magnitude currently found in lithium-ion battery technologies.

3:00 PM

(ENERGY-133-2010) Quantitative Characterization of Lithium Ion Batteries by Microscopic Techniques

T. Bernthaler, C. N. Hafner*, R. Löffler, A. Nagel, V. Pusch, G. Schneider, Hochschule Aalen, Germany

Lithium ion batteries are the most attractive candidates for mobile electronic devices and automotives applications. The functionality of Li ion batteries bases on the change of active materials due to diffusion processes. Electrochemical and physical characterization techniques are well advanced and published. Unlike these techniques the microscopic visualization and quantification of the microstructure of the electrode materials are not state of the art. However, parameters of cell performance and various aging mechanisms depend strongly on the appearance and changes in the microstructure. Hence, the investigation and quantification of microstructures is of increasing importance for the understanding of battery materials. We present the potential of the combined microscopic techniques nano 3D-computed tomography, optical microscopy, scanning electron microscopy and image analysis to visualize and characterize cell designs and the microstructure of active materials. The process how to prepare and investigate Li ion batteries by these techniques will be described. To achieve specific microstructural features of the active materials the method of the quantitative microstructure analysis will be explained. Important parameters like the volume fraction of different phases, homogeneity, pores, cracks, grain size and shape distribution and specific surfaces and interphases will be discussed.

3:40 PM

(ENERGY-134-2010) Microstructural Control and Characterization of BICUVOX Ceramics

S. Razmyar*, K. Sabolsky, E. M. Sabolsky, West Virginia University, United States

The widespread commercialization of solid-oxide fuel cells (SOFCs) and solid-oxide electrolyte cells (SOECs) is primarily limited by materials degradation issues related to the required high temperature operation (>800C). Research is required to develop the next generation of solid ionic electrolytes for these applications that display ionic conductivities exceeding 10-2 S/cm at temperatures <800C. The typical approach is through the doping of various fluorite, perovskite, and pyrochlore structured materials to alter ionic vacancy concentration and order. Relatively few researchers have explored methods of manipulating the microstructure of bulk ceramic oxides to control diffusional kinetics. The proposed approach may lead to electrolyte ceramics with enhanced ionic conduction and mechanical strength. Research on controlling grain orientation and grain growth kinetics of Bi2CuxV1-xO5.5-z (BICUVOX) will be presented. Discussions will focus on the effect of processing variables, like liquid phase content, powder characteristics and thermal conditions on density, grain growth, orientation, and mechanical strength.

4:20 PM

(ENERGY-135-2010) Texture Development during Hot Deformation of Bismuth Telluride and Bismuth Telluride based Composites (Invited)

R. Srinivasan*, Wright State University, United States; N. Gothard, J. Spowart, Air Force Research Laboratory, United States

Bismuth telluride (BT) has the highest Seebeck coefficient near room temperature making it the best candidate for refrigeration and energy conversion processes near RT. The crystallographic structure of this material is stacked planes following the sequence –[-Te-Bi-Te-Bi-Te-]n– in the “c” direction. The Bi and Te layers are covalently bonded, and adjacent Te layers have weak secondary bonds. Basal cleavage and basal slip are the primary fracture and deformation modes. This paper presents development of texture during hot deformation of BT and BT-carbon composites with C60 and nano-graphene. A variety of processing techniques, including extrusion, rolling, and powder sintering will be examined with aim of producing bulk textured ultrafine grained materials.

Nuclear

Modeling and Simulation

Room: Dunes 1&2

Session Chairs: Alex Larzelere, U.S. Department of Energy; Marius Stan, Los Alamos National Laboratory

1:40 PM

(ENERGY-136-2010) Nuclear Energy Advanced Modeling and Simulation: An Introduction (Invited)

A. Larzelere*, U.S. Department of Energy, United States

The United States and the world is facing a growing challenge about how to provide the energy required to maintain and grow the economic output of the world’s countries. Providing that energy is important because increased economic output correlated to improved standard of living and reduces the likelihood that countries will go to war. As the United States considers its energy future, think about its “energy security” in three terms. The first is “national security” and the need to use energy sources that will not require military intervention to protect the sources or their supply routes. The second is “economic security” and the fact that energy should be affordable (not necessarily cheap) and reliable (to avoid market uncertainties). The last consideration is “environmental security” and the need to obtain energy sources that are friendly to the environment, particularly in the light of the threat of global climate change. There are many forms of alternative and renewable energies that can improve U.S. energy security. One of those is nuclear energy. To increase the usage of nuclear energy, and thus energy security, certain technology issues must be addressed. These include; safely extending the life of the existing reactors, improving the pace and cost of deployment of the next generation reactors, developing innovative uses of the energy from nuclear reactors, improving the pace and cost of deployment of the next generation reactors, developing innovative uses of the energy from nuclear reactors, and appropriately dealing with the waste issue. All of this must be done in ways that avoid increasing the risk of proliferation. Advanced modeling and simulation can contribute to improved understanding of all of these technology areas. Advanced capabilities provide modeling and simulation that is three dimensional, high resolutions, based on first principle science, and include coupled physics. These features require the use of high performance computing. Advanced modeling and simulation will be coupled with theory and experiments and used to help understand "what happens" during complex physical processes under condition that not normally visible (like in a nuclear reactor). The creation of advanced modeling and simulation capabilities requires a close coupling of many elements of an applications code. In particular, building the capability requires the appropriate linkage of models that describe atomistic level behaviors, through the mesoscale, to the continuum scale. Doing this allows scientists and engineers to usethe capabilities to predict system performance and address nuclear energy technology issues. The talks following this introduction will focus on the creation of models at the atomistic and meso scales that are critical to understand material performance that eventually links to the high engineering scale modeling and simulation.

2:00 PM

(ENERGY-137-2010) Advanced Models and Simulations of Nuclear Fuels (Invited)

M. Stan*, Los Alamos National Laboratory, United States

Computer simulations are currently used to predict nuclear reactor phenomena such as neutron and heat transport, fluid dynamics, and the effect or radiation on the properties of nuclear fuel elements and structural materials. An important component of the complex simulation methodology is predicting the performance of nuclear fuel elements. After a brief review of world-wide status of fuel performance codes, the presentation focuses on recent Finite Element simulations of coupled heat transfer, chemical species diffusion and thermal expansion of UO2+x fuel elements with metallic clad. The continuum simulations incorporate multi-scale models and simulations of fuel properties, such as atomistic (Molecular Dynamics) models of point defect concentration and meso-scale (Phase Field) simulations of gas bubble formation. The continuum, coupled simulations demonstrate that including the dependence of thermal conductivity and density on local composition (oxygen and fission products content) leads to changes in the predicted centerline temperature that exceed 5%. The final part of the talk is dedicated to a discussion of national and international strategies for developing advanced, innovative models and high performance simulations for nuclear energy applications.

2:20 PM

(ENERGY-138-2010) Center for Materials at Irradiation and Mechanical Extremes (Invited)

M. Nastasi*, Los Alamos National Laboratory, United States

Our new Energy Frontier Research Center (EFRC), entitled Center for Materials at Irradiation and Mechanical Extremes responds to two grand challenges put forward by Basic Energy Sciences: How do we design and perfect atom and energy-efficient syntheses of revolutionary new forms of matter with tailored properties?; and How do we characterize and control matter away-especially very far away-from equilibrium? This Center recognizes that the challenge to developing materials with radically extended performance limits at irradiation and mechanical extremes will require designing and perfecting atom- and energy-efficient synthesis of revolutionary new materials that maintain their desired properties while being driven very far from equilibrium. We have developed a set of common science issues that will drive our science focus and serve as the unifying foundation of this center. These scientific issues include: 1) Absorption and recombination of point and line defects at interface; 2) Morphological and chemical stability of interfaces; 3) Interface-driven mechanical response. By addressing these issues we will develop a fundamental understanding of how atomic structure and energetics of interfaces contribute to defect and damage evolution in materials, and use this information to design extreme environment-tolerant materials via atomic scale design of interfaces.

2:40 PM

(ENERGY-139-2010) Defect Dynamics of Irradiated Microstructures (Invited)

T. Arsenlis*, M. Rhee, G. Hommes, Lawrence Livermore National Laboratory, United States

The desire to increase the utilization of fuel in nuclear reactor cores is driving a renewed interest in modeling the degradation of materials in such environments in hope of producing predictive models of materials performance and life limits. Under these conditions, material microstructures may develop second phase precipitates, noble gas bubbles, prismatic dislocation loops, vacancy clusters, and other nano-scale defect structures. Dislocation dynamics simulation tools, designed to simulate the interaction of dislocations leading to strength and strain hardening, can be simply augmented to create defect dynamics simulation tools by including the enumerated irradiation defects through the use of Eshelby inclusions. In these defect dynamics simulations, the defects interact through their elastic strain fields and though a series of rules detailing their reaction at defect-defect intersections. Such tools can be used to simulate the effect of dislocation networks on the microstructural evolution during irradiation and the effect of irradiated microstructures on the evolution of dislocation networks during mechanical loading. Details of the implementation of Eshelby inclusions into the Parallel Dislocation Simulator (ParaDiS) code project will be discussed, and initial results of prototypical strain hardening simulations in the presence of prismatic loops and volumetric inclusions will be presented. Initial functional forms for defect-based coarse grained models of irradiation hardening/embrittlement will be offered.

3:00 PM

(ENERGY-140-2010) A Perspective on Mesoscale Modeling of Irradiated Nuclear Reactor Materials (Invited)

A. El-Azab*, Florida State University, United States

Future nuclear reactors will be designed for prolonged lifetime, improved economics and considerable safety margins. To enable these design goals, robust predictive capabilities must be developed to understand the behavior fuel and structural materials in the aggressive reactor environment and to integrate the related materials models into the reactor design tools. Modeling of the mesoscale response of materials is a central part of such predictive capabilities. Basically, at this scale, the materials complexity reveals itself in the form of coupled compositional and microstructural heterogeneities that dominate the materials response. In this talk, we highlight a generalized mesoscale modeling framework for coupled microstructure and compositional evolution in oxide and alloy fuels under irradiation. This framework, which is based on non-equilibrium thermodynamics of materials and the diffuse interface concept of microstructure evolution in materials, is equally valid for structural ceramics and alloys. Sample results are given for the irradiation-induced void and gas-bubble nucleation and growth, dislocation loop formation and component redistribution in irradiated fuels. These results show that the current approach is capable of handling the complexity of the material response at the mesoscale. The results also demonstrate that breakthroughs in understanding and predicting the macroscale behavior of irradiated fuel and structural materials can only be made via success at the mesoscale level. The talk concludes with the author's perspective on future research directions in this important area.

3:40 PM

(ENERGY-141-2010) Fission Gas Behavior in UO$_2$: Atomistic Simulation of Multidimensional Defects

C. Stanek*, D. Andersson, B. Uberuaga, P. Nerikar, Los Alamos National Laboratory, United States

As is well known, the performance of nuclear fuel is strongly related to the behavior of fission gases, such as xenon. If fission gases are retained, the fuel swells and is increasingly likely to mechanically interact with the clad. Whereas, if the fission gases are released, the plenum pressure increases. Both situations increase to probability of clad failure, and therefore must be understood for fuel qualification. The complexity of fission gas behavior has to date prevented such an understanding. In this talk, we present recent simulations of Xe in UO_2 that contribute to improved understanding of fission gas behavior. Specifically, we have built upon previous atomistic simulation studies of Xe bulk diffusion to consider the effects of grain boundary structure of gas transport. By considering the relationship between 1, 2, and 3 dimensional defects (i.e. dislocations, grain boundaries and bubbles) with zero dimensional defects (i.e. fission gas atoms), we are able to simulate fission gas transport as a function of microstruture. Such insight can subsequently be used to improve higher length scale models – an example of which will be discussed.

4:00 PM

(ENERGY-142-2010) Activation energies for Xe transport in $UO_{2\pm x}$ from density functional theory calculations

D. Andersson*, P. Nerikar, B. Uberuaga, C. Stanek, Los Alamos National Laboratory, United States

The formation and redistribution of fission gases are critical determinants of nuclear fuel performance and in particular limit the extent of burnup. One of the controlling steps for evolution of fission gas micro-structures is diffusion of individual gas atoms through the fuel matrix to existing bubbles or grain boundaries (sinks). Here we have studied the bulk diffusion mechanisms of Xe by calculating the corresponding activation energies as function of the $UO_{2\pm x}$ stoichiometry using density functional theory (DFT) methods. Estimating the activation energy involves determining Xe migration barriers as well as the thermodynamics of Xe trap sites in $UO_{2\pm x}$ and their interactions with the U vacancies that enable Xe in trap sites to move. We present results for all these components. Due to the complex nature of the clusters of point defects that interact with Xe atoms, the DFT based modeling is inevitably associated with uncertainties that in some cases may be rather significant. In order to mitigate this issue, we have identified systematic errors, after which we categorize the most probably diffusion mechanisms. In order to achieve self-consistency and assess the accuracy of our conclusions, this exercise is complimented by re-analysis of key experimental data within the framework of proposed diffusion models.

Hydropower

Materials Challenges in Hydro and Geothermal Energy

Room: Sea Oats
Session Chairs: Brenda Garcia-Diaz, Savannah River National Laboratory; Hidda Thorsteinsson, U.S. Dept. of Energy

1:40 PM

(ENERGY-143-2010) Ocean Thermal Energy Conversion: Heat Exchanger Evaluation and Selection (Invited)

M. A. Laboy*, Offshore Infrastructure Associates, Puerto Rico; O. E. Ruiz, University of Puerto Rico - Mayaguez Campus, Puerto Rico; J. Martí, Technical Consulting Group, Puerto Rico

This study summarizes available data on heat exchanger requirements for closed-cycle OTEC power systems obtained during over thirty years of R&D work and technology demonstration programs, and presents how these requirements can be met using commercially-available heat exchangers used today in other applications by a variety of industries. The study focuses on the following design criteria: configuration (shell-and-tube, compact-type, and others), process performance, surface enhancement, corrosion resistance, biofouling control, manufacturability, ease of operation and maintenance, and over-all cost-effectiveness. Selection of the appropriate working fluid will also be discussed. Data to be evaluated include previously developed power system designs such as those completed during the 1970's and 1980's by GE, JHU/APL, ANL, and engineering reports from OTEC technology demonstration programs such as the Nauru, Mini-OTEC and OTEC-1 test projects. A critical performance assessment is made between the use of stainless-steel plate heat exchangers and aluminum-brazed plate-fin heat exchangers in the context of present day technology. Alternatives to mitigate and control the adverse effects of biofouling are discussed.

2:00 PM

(ENERGY-144-2010) Optimal Operation of Cascaded Hydroelectric Plants in Energy Market with Considering Value of Water (Invited)

M. Heidarizadeh*, M. Aghamohammadi, power and water university of Technology, Iran, Islamic Republic of; T. Akbari, tehran university, Iran, Islamic Republic of; M. Ahmadian, power and water university of Technology, Iran, Islamic Republic of

The aim of this paper is to propose a new method for optimal operation of cascaded hydroelectric plants in energy market with considering value of water. In this method we have assumed that hydroelectric plants are providing the major part of generated energy, and then price of energy will change regarding the amount of water behind dam. Since increment in this amount will result in higher efficiency of plant and change in power price, the operator should regard these parameters to have optimal operation. In this paper we have studied two scenarios. In the first one we have assumed that hydroelectric plants have no effect on prices. In the second scenario we have assumed that there would be the possibility of price change regarding the amount of water behind dams. In this article the operation period is considered to be one year and time intervals are one month. To solve the problem we have used GAMS software and the proposed method is used on a system with 3 hydroelectric dams.

2:20 PM

(ENERGY-145-2010) Advanced Composite Materials for Tidal Turbine Blades

M. Tupper*, M. Hulse, J. Cronin, W. Francis, CTD, United States

The energy potential of harnessing the kinetic energy of the world's ocean and tidal currents is part of the US's renewable energy plan. Technologies that improve the performance and reliability of marine current energy systems are needed. Marine current energy systems convert kinetic energy of moving tides and currents into electrical energy via underwater turbines. These turbine blades are designed to withstand the challenges of the marine environment including high hydrodynamic forces, corrosion due to salt water, and erosion due to cavitation, and impact from suspended particle. Advanced composites are attractive for constructing tidal turbine blades. However performance improvements are needed regarding impact-damage and cavitation-erosion resistance. If not properly addressed, this could dramatically reduce the size, efficiency, reliability and life-span of tidal turbines thereby reducing the viability of marine current energy systems. Recent work focused on composite ship propellers have shown substantially improved cavitation-erosion and impact-damage resistance in comparison to industry-standard materials while also possessing necessary mechanical properties and processing characteristics. Adaptation of these cavitation resistant composite materials can significantly improve the performance and economic feasibility of ocean tidal systems.

2:40 PM

(ENERGY-146-2010) Effect of delta ferrite on impact properties of low carbon 13Cr4Ni martensitic stainless steel

P. Wang*, S. Lu, N. Xiao, D. Li, Y. Li, Institute of Metal Research,Chinese Academy of Sciences, China

The effect of delta ferrite on impact properties of 13Cr4Ni martensitic stainless steel was studied by instrumented impact, SEM and EDS. The experimental results indicated the presence of delta ferrite did not change the upper and lower shelf energy of the steel, however, lowered the impact energy remarkably during the ductile-brittle transition temperature range and raised the ductile to brittle transition temperature of the material. At 0 centigrade, which is in the ductile-brittle transition temperature range, the presence of 7.8% delta ferrite lowered the crack initiation and propagation energy of the impacting and changed the fracture mode from dimple to quasi-cleavage. It is suggested that in the transition temperature range the cracks are initiated in the delta ferrite, which lowers the maximum load and crack initiation energy. Additionally, when the cracks initiating in delta ferrite extend to the boundaries between the delta ferrite and the matrix, they trigger brittle fracture in the tempered martensite matrix, which decreases the crack propagation energy dramatically. The presence of delta ferrite deteriorates the material's toughness and decreases the life of the hydraulic turbine which is made of 13Cr4Ni martensitic stainless steel, therefore proper Ni and Cr equivalent should be controlled to avoid the delta ferrite.

3:00 PM

(ENERGY-147-2010) Martensitic Stainless Steel 0Cr13Ni4Mo for Hydraulic Runner (Invited)

Y. Li*, D. Li, Institute of metal research, Chinese Academy of Sciences, China

Three Gorges hydraulic runner is the largest size in the world and its weight is nearly 400 tons. It consists of the top crown and the lower ring through the blades which are welded together. The materials are 0Cr13Ni4Mo which is precipitation hardening martensitic stainless steel. The chemical composition requirements, heat treatment specification and microstructure of martensitic stainless steel 0Cr13Ni4Mo were described in detail. 0Cr13Ni4Mo stainless steel is mainly used for normalizing and tempering conditions. Using reasonable content of alloying elements and adjust the Ni/Cr equivalent proportion, the Delta-Ferrite can be avoid in the microstructure. Single normalizing and double tempering are recommended for the heat treatment system. The normalizing microstructure consists of 100% the lath martensite. The final microstructure in 0Cr13Ni4Mo stainless steel is tempered martensite and a certain amount of inversed austenite which have an excellent comprehensive mechanical properties and good weldability.

3:40 PM

(ENERGY-148-2010) Alloy Testing, Selection, and Condition Monitoring Challenges for Geothermal Energy Systems

B. Amend*, DNV Columbus, Inc., United States

Geothermal fluids comprise a wide range of fluid compositions, temperatures and pressures and can include some of the most corrosive naturally occuring water compositions known to man. It is important to consider probable alloy degradation mechanisms, degradation rates and, related degradation detection and monitoring methods when engineering geothermal energy production and utilization systems. However, the diversity of geothermal fluid characteristics makes it challenging to select cost-effective metallic materials of construction. This presentation will address considerations in the testing, selection, and condition monitoring of metallic materials of construction in geothermal energy production. The preferred process of materials selection consists of a multi-step procedure that includes consideration of normal, transient, and abnormal operating conditions, the effects of component manufacturing and fabrication on corrosion resistance, the effects of various degradation mechanisms on system safety and reliability (for example, susceptibility to failure by leak versus rupture) and the ability to detect and monitor those various forms of degradation in service. Examples of geothermal enegy system component failures resulting from oversights in the material selection and/or condition monitoring process will be included.

4:00 PM

(ENERGY-149-2010) Experience with the Development of Advanced Materials for Geothermal Systems

T. Sugama, T. Butcher*, Brookhaven National Laboratory, United States

Over the past ten years, the emphasis of the geothermal material programs at DOE Brookhaven National Laboratory (BNL) was directed towards resolving the material-related problems confronting the geothermal-drilling and -power plant industries in the conventional natural hydrothermal system. In the drilling fields, BNL developed high temperature, highly chemical-resistant well cementing materials that withstood in the hydrothermal environment containing >10,000 ppm CO2 and H2S (pH ~3.0) at 300°C. As a result, this material offered a significant extension of lifespan of well-casing cement, leading to saving the substantial amount of well maintenance cost. Most recent work was devoted to designing cost-effective inorganic polymer-based cementitious materials by using recycled industrial byproducts, such as fly ash and slag. Subsequently, new-type material called "Geopolymer," possessing advanced properties such as great adherence to well rock surfaces and readily controlled setting behavior at high temperature. This information urged us to evaluate and validate its potential for use as sealing material in Enhanced Geothermal Systems (EGS). In the energy conversion fields, our focus centered on developing advanced coating material systems, which provide upgraded corrosion-, erosion-, and fouling-prevention performances for carbon steel- and aluminum-based power plant components including wellhead, heat exchangers, condensers, and steam separators in very harsh geothermal environments. As a result, several coating systems were developed. Among these were the highly thermal conductive, self-healing, multifunctional coatings for wellhead and heat exchanger at hydrothermal temperatures up to 250°C, the self-assembling nanocomposite coating for air-cooled condensers, and the low friction, wear resistant coating for steam separators.

4:20 PM

(ENERGY-150-2010) Novel High Temperature Materials Enabling Operation of Equipment in Engineered Geothermal System Wells

M. Tupper*, C. Hazelton, M. Hooker, K. Kano, L. Adams, Composite Technology Development, Inc., United States

Geothermal energy is a key renewable source of energy, which unlike wind and solar power, is not affected by changing weather and is always available to meet power demands. For geothermal energy to be widely utilized, deeper wells to reach hot, dry rock, located beneath the Earth's surface are required. Water will be introduced to create a geothermal reservoir or an Enhanced Geothermal System (EGS). EGS reservoirs are at depths of up to 10 km, and the temperatures at these depths are limiting the use of available down hole equipment. Down-hole submersible pumps are a key component for large-scale power generation from geothermal resources. Both Hydrothermal and Enhanced Geothermal Systems require a robust serviceable pump capable of bringing heat to the surface. The critical attributes of such a pump are temperature tolerance and low service needs. Development of geothermal will depend on the flow of high temperature resources. At that point, reliability and robustness will be key operating features. Existing pumps are limited to 190C, preventing high value hydrothermal resources in the 190 to 220C range from being developed. Novel high temperature composite materials are being developed and demonstrated for use in new ESPs that can meet the challenging demands of EGS wells and can accelerate the exploitation of this large renewable source of energy.

Recent Developments

Tuesday, February 23, 2010

7:00 PM

(ENERGY-P024-2010) Mechanical and Rheological Properties of Blends of Poly (phenylene sulfide) and Liquid Crystalline Polymers: The use of Recycled Poly (ethylene terephthalate)

H. Shaban*, Kuwait University, Kuwait

A thermotropic liquid crystalline polymer (LCP), based on the modification of recycled poly (ethylene terephthalate) with 4-acetoxy benzoic acid was synthesized. A block copolymer between poly (phenylene sulfide) (PPS) and the synthesized LCP, intended to be used a compatibilizer, was also developed. Blends of PPS and the LCP were prepared using a co-rotating twin-screw extruder. The rheological and mechanical properties of the neat and blended polymers were analyzed. The viscosity of the compatibilized in situ composite decreased in the presence of the compatibilizer, which is mainly due to the fibrous structure of the LCP at high shear rates. The mechanical properties of the compatibilized blends increased when a proper amount of the compatibilizer was added. This is attributed to fine fibril generation induced by the addition of PPS-β-LCP.

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*** Denotes Presenter**

2010-2011 Meetings & Expositions of The American Ceramic Society

May 10-12, 2010
Structural Clay Products Division Meeting
Gettysburg, Pennsylvania, USA

May 16-19, 2010
Glass & Optical Materials Division Spring Meeting
Radisson Hotel Corning
Corning, New York, USA
www.ceramics.org/gomd2010

June 21-22, 2010
Ceramic Leadership Summit
Hyatt Regency Baltimore
Baltimore, Maryland, USA
www.ceramics.org/ceramicsummit2010

July 11-13, 2010
Cements Division & Center for Advanced Cement-Based Materials Meeting
Purdue University
West Lafayette, Indiana, USA
www.ceramics.org/cements2010

October 17-21, 2010
Materials Science & Technology 2010 Conference & Exhibition (MS&T'10) & ACerS 112th Annual Meeting
George G. Brown Convention Center
Houston, Texas, USA
www.matscitech.org

January 19-21, 2011
Electronic Materials & Applications
Royal Plaza in the Walt Disney® World Resort
Orlando, Florida, USA

January 23-28, 2011
35th International Conference & Exposition on Advanced Ceramics & Composites
Hilton Daytona Beach Resort & Ocean Center
Daytona Beach, Florida, USA

August 1-2, 2011
Ceramic Leadership Summit
Hyatt Regency Baltimore
Baltimore, Maryland, USA

October 16-20, 2011
Materials Science & Technology 2011 Conference & Exhibition (MS&T'11) & ACerS 113th Annual Meeting
Greater Columbus Convention Center
Columbus, Ohio, USA
www.matscitech.org

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