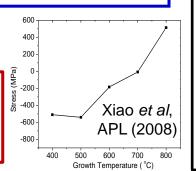
Grain Boundary Induced Stresses in Nanocrystalline Ceramic Coatings and Thin Films

Brian W. Sheldon, Janet Rankin (Brown University), Barbara Walden (Trinity College)

Nanocrystalline Diamond

Stress During
CVD Growth:

Large Impact of Grain Bdry Chemistry & Structure

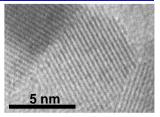


In situ film stress from optical curvature measurements film substrate

Non-Stoichiometric Oxides

Stress Due to O
Variations in CeO_{2-X}

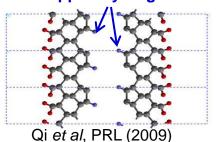
Grain Bdry
Contributions
Dominate Stress

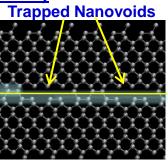


Nanocrystalline CeO_{2-X} deposited from Ce(thd)₄

DFT Calculations (w. Yue Qi at GM)

Trapped Hydrogen





Milas et al, JAP (2011)

Ceria at 500 C:

Oxidation - O₂
Reduction - CO / CO₂

reduction

oxidation

oxidation

reduction

oxidation

Time(sec)

x 10

Large Local Stresses
(up to 10 GPa !)
in Space Charge Layers

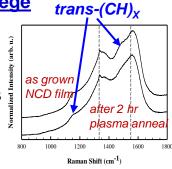
Bulk
Grain

substrate

Sheldon, PRL (2011)

Trinity College

- faculty involved in research (Raman)
- Trinity undergrads working at Brown



Broader Impacts

General Motors

- interest in low friction NCD coatings
- DFT (see above)
- use of GM facilities

<u>Institute National Polytechnique –</u> Toulouse (France)

- H and OH induced stresses in protective alumina coatings (on Ti alloys)
 - Soni et al, ECS Trans (2010)
- extensive student and faculty exchanges

DMR-Award 0805172