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AEROSPACE MATERIALS FOR EXTREME ENVIRONMENTS

Date: 7 March 2013

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Program Officer
AFOSR/RTD**

Air Force Research Laboratory

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2013 AFOSR SPRING REVIEW



NAME: AEROSPACE MATERIALS FOR EXTREME ENVIRONMENTS

BRIEF DESCRIPTION OF PORTFOLIO:

To provide the fundamental knowledge required to enable revolutionary advances in future Air Force technologies through the discovery and characterization of materials that can withstand extreme environments.

LIST SUB-AREAS IN PORTFOLIO:

- Theoretical and computational tools that aid in the discovery of new materials.
 - Ceramics
 - Metals
 - Hybrids (including composites)
- Mathematics to quantify the microstructure to Predictive materials Science
- Physics and chemistry of materials in highly stressed environments
- Experimental and computational tools to address the complexity of combined external fields at extreme environments.



OUTLINE



I. Predictive Materials Science

Bulk Metallic Glasses

Carbides (SiC, TaC, Ta₄C)

Textile Based Hybrid Composite

II. Materials Far from Equilibrium

Micro-Architected Surfaces

Surface Catalysis at Extreme Environment

III. Challenges, Motivations and New initiatives.

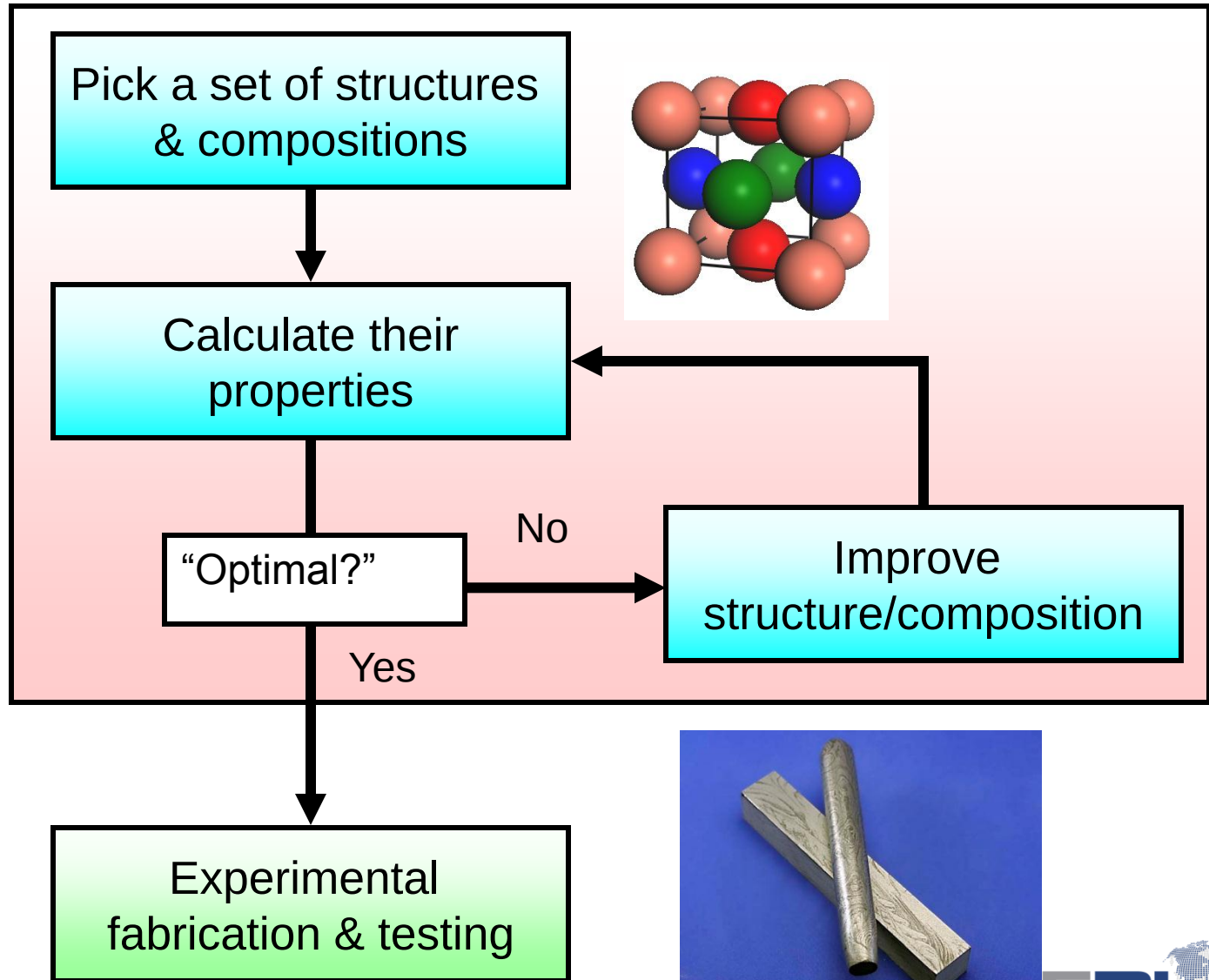


"The Dream:"

Computational Material Design



W. Windl (OSU), K. Flores (WASHINGTON U.), D. Hoffmann (CALTECH), E. Marquis (U. MICHIGAN)



Computer



Lab or Fab





Ab-Initio Calculations

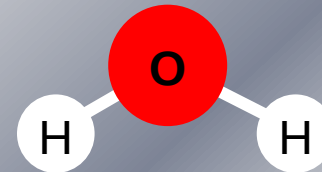


W. Windl (OSU), K. Flores (WASHINGTON U.), D. Hoffmann (CALTECH), E. Marquis (U. MICHIGAN)

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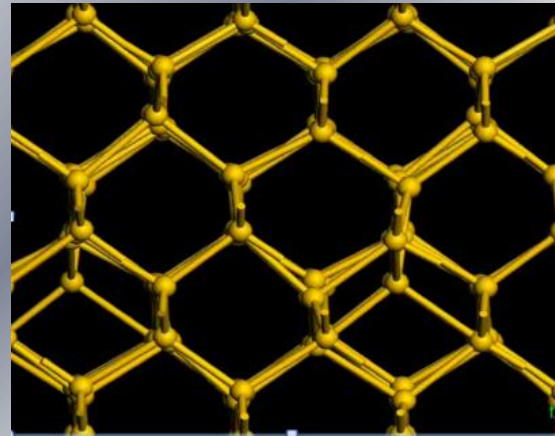


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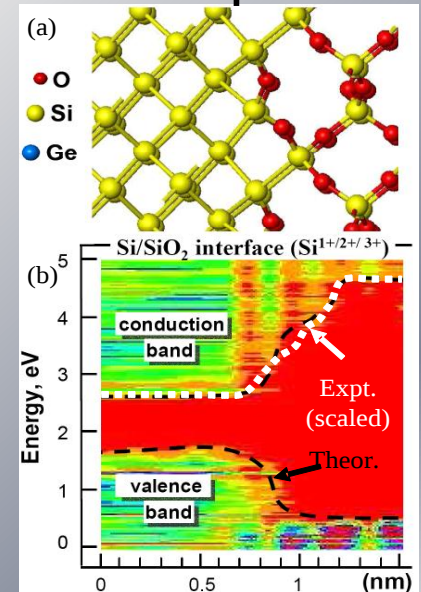


Structure,
Energy

Band structure
EELS spectra



Kinetic parameters
Thermal properties
Mechanical prop's



**Ab Initio
Code**

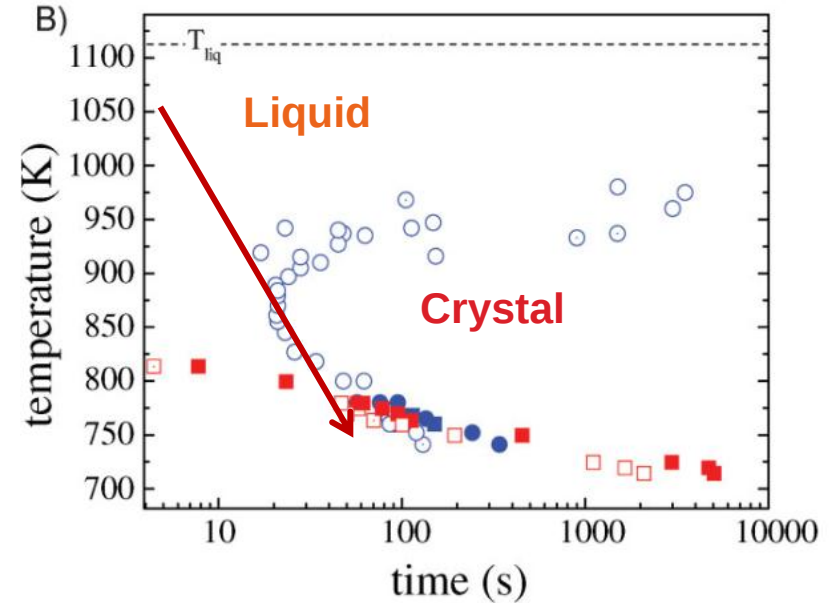
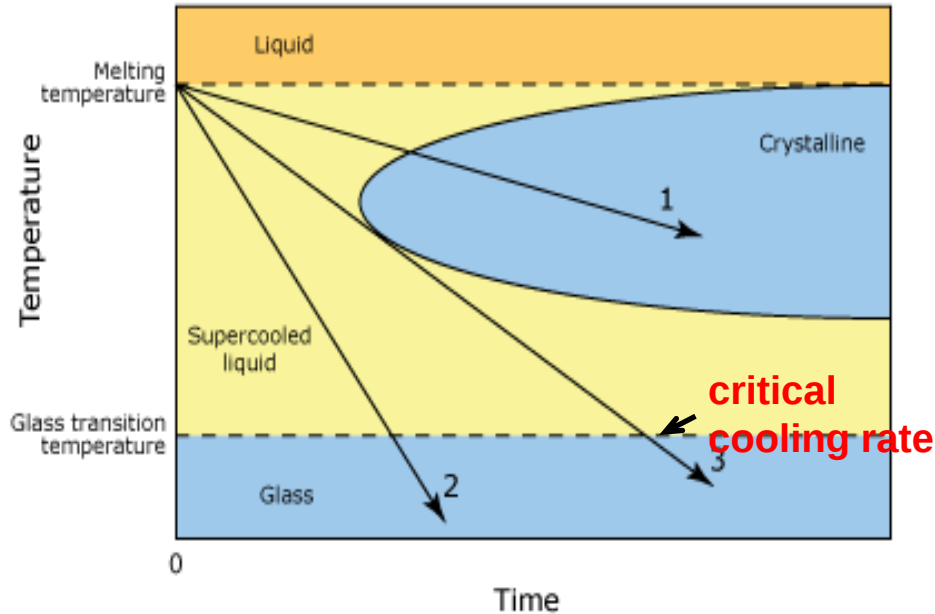
$$H\psi = E\psi$$



Calculating Glass-Forming Ability



W. Windl (OSU), K. Flores (WASHINGTON U.), D. Hoffmann (CALTECH), E. Marquis (U. MICHIGAN)



Crystallization inhibitors:

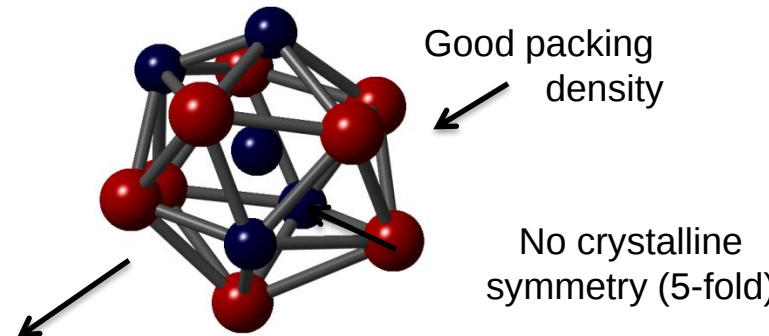
1. **Driving Force:** Icosahedra
2. **Kinetics:** Viscosity (fragility)

Direct Measurement:

Critical Cooling Rate

- Not computationally feasible
- Real time: 1 ms
- 20 CPUs: **200 Years**

Stabilize liquid;
don't lead to crystal nuclei



Frank, F. C. (1952).



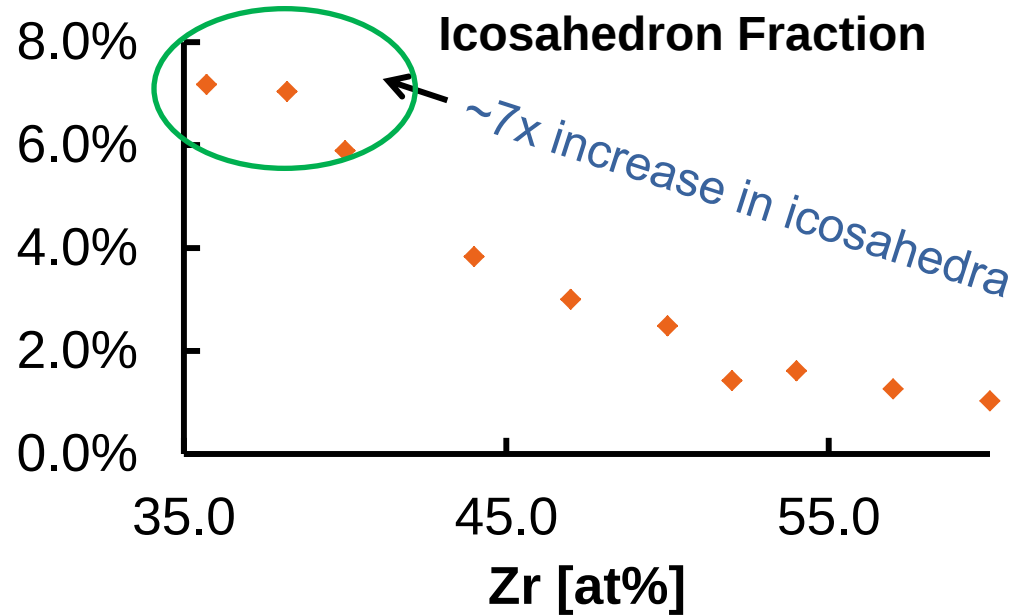
Interatomic Potentials



W. Windl (OSU), K. Flores (WASHINGTON U.), D. Hoffmann (CALTECH), E. Marquis (U. MICHIGAN)

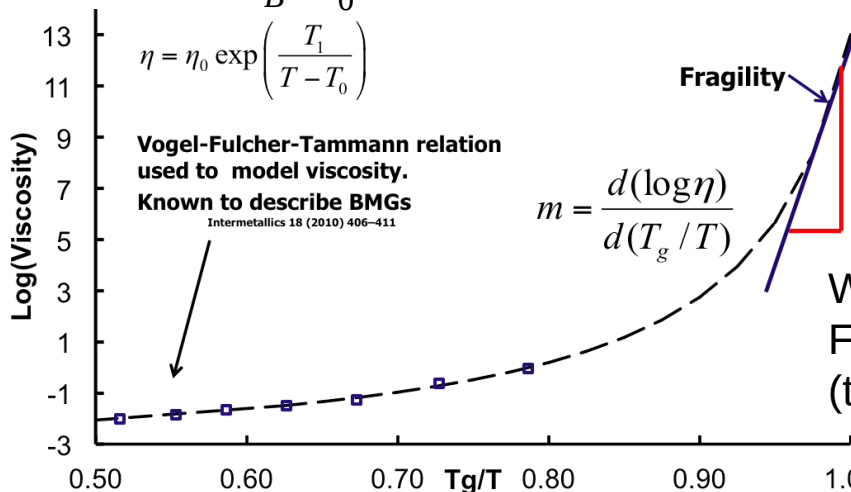
	Ag	Al	Au	Be	Ce	Co	Cu	La	Mg	Nb	Ni	Ta	Ti
Al	9.094												
Au	12.056	6.060											
Be	0.710	1.067	0.509										
Ce	4.407	2.196	3.590	1.246									
Co	5.400	1.264	5.946	0.509	1.657								
Cu	3.049	3.984	7.424	0.579	2.045	4.814							
La	2.559	3.280	1.935	0.716	1.827	1.345	1.887						
Mg	1.021	1.536	0.552	1.386	0.807	0.900	1.861	0.746					
Nb	0.694	1.213	1.041	0.667	6.288	2.122	0.611	2.674	0.194				
Ni	6.836	4.069	5.339	0.494	1.812	7.348	6.123	2.425	1.129	5.539			
Ta	2.400	1.138	2.250	0.432	1.599	2.288	1.457	4.563	1.408	2.400	3.114		
Ti	5.334	1.945	2.925	1.181	2.924	3.641	2.740	3.794	0.539	2.908	1.526	2.152	
Zr	2.721	1.500	2.403	0.924	3.840	3.089	3.286	3.851	3.618	2.371	1.790	2.225	8.558

atomistics.osu.edu

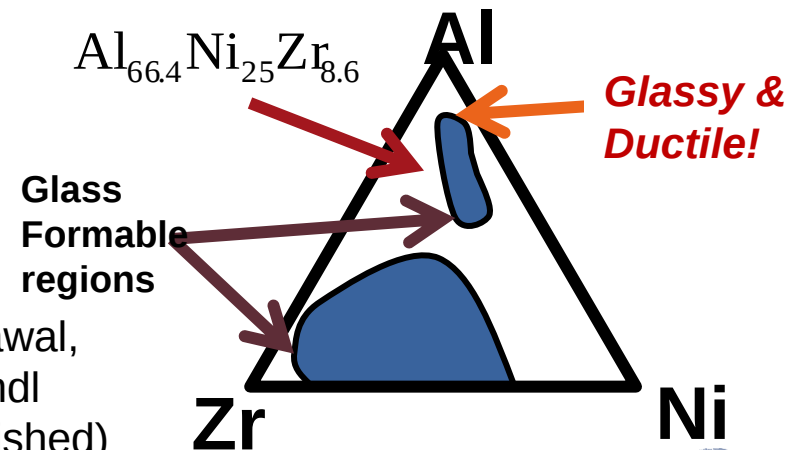


Chosen Method: Green-Kubo

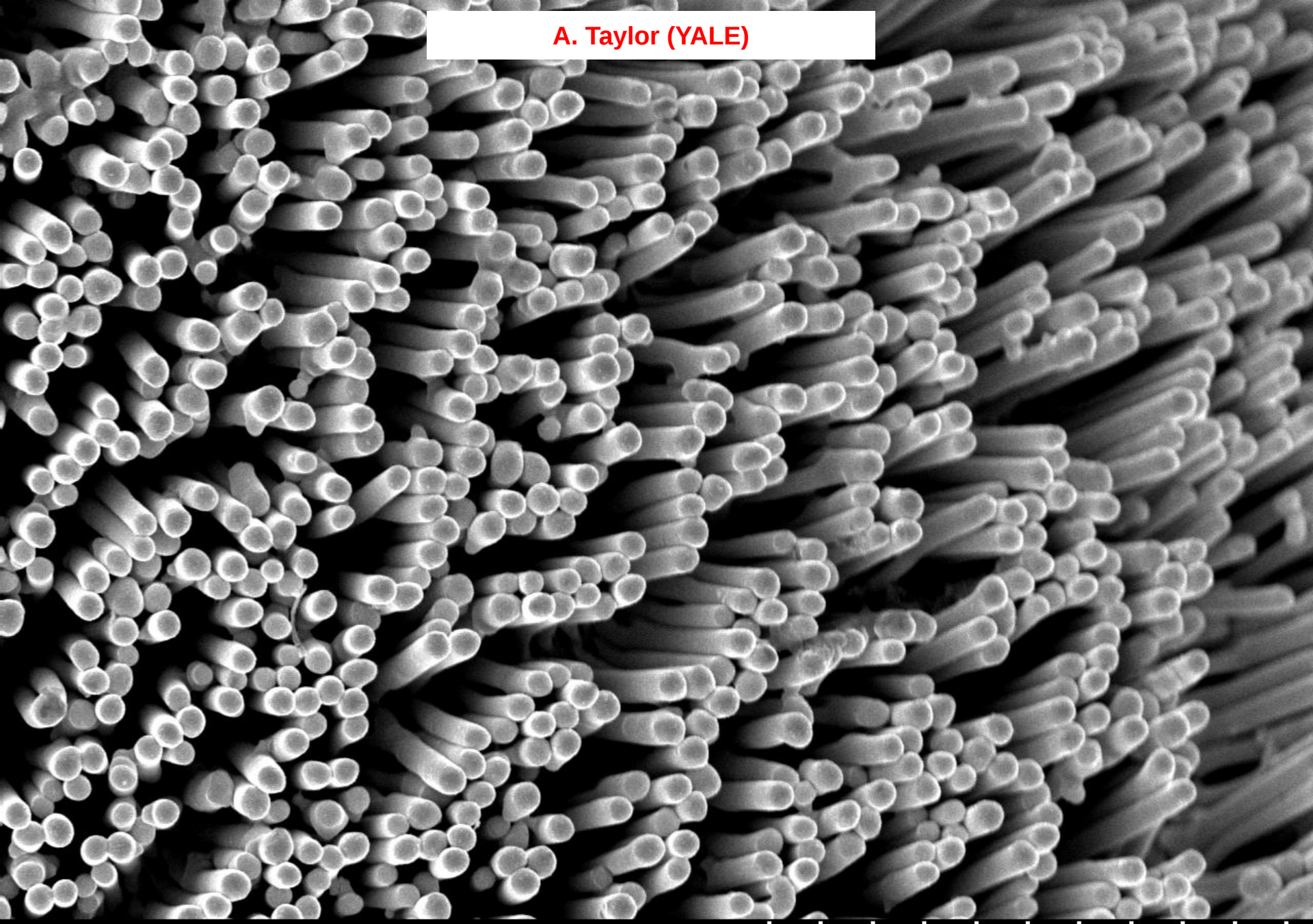
$$\eta = \lim_{t \rightarrow \infty} \frac{V}{k_B T} \int_0^t \langle P_{\alpha\beta}(t_0 + s) P_{\alpha\beta}(t_0) \rangle ds$$



Ward, Agrawal, Flores, Windl (to be published)



A. Taylor (YALE)



Yale 10.0kV 5.9mm x10.0k SE(M)

5.00um



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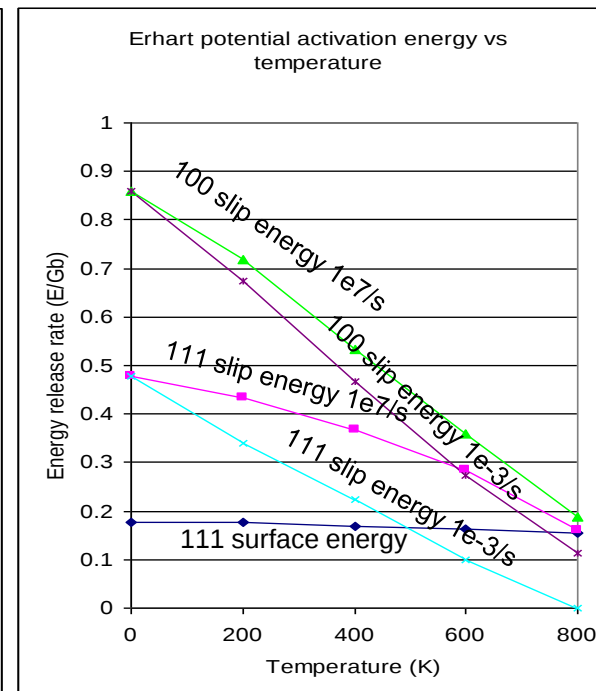
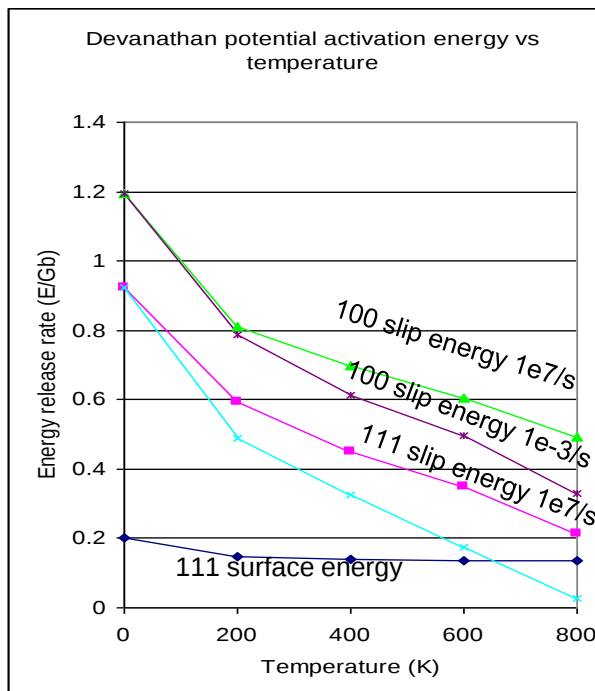
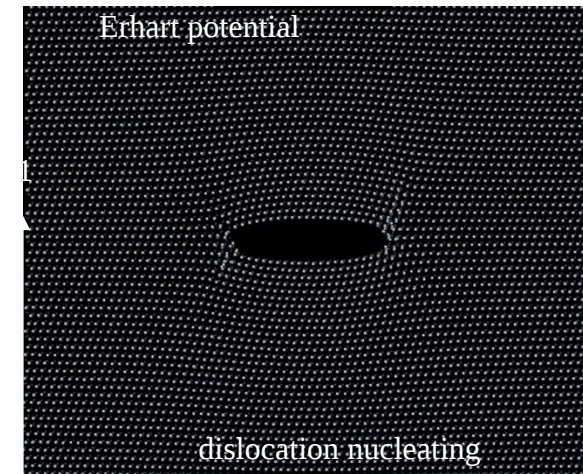
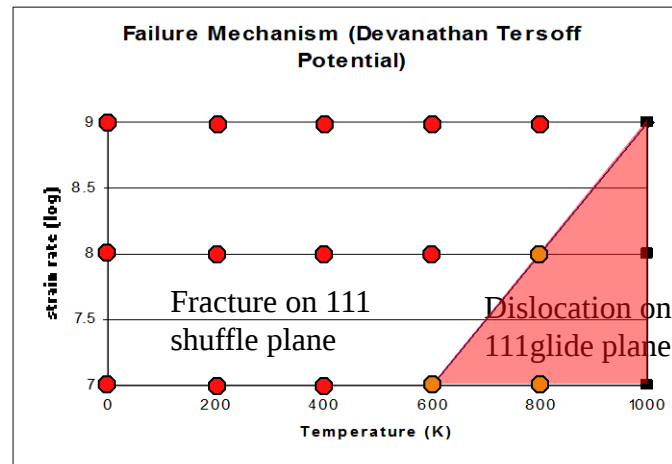
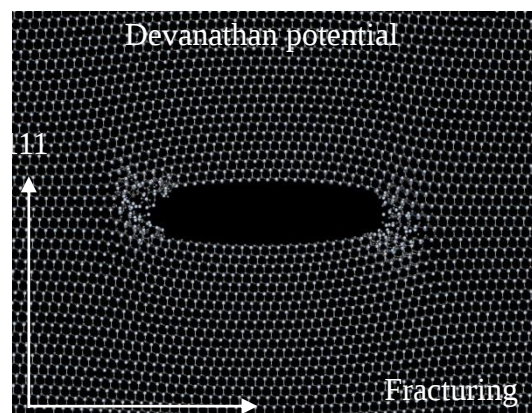
III. Challenges, Motivations and New initiatives.



Direct MD prediction compared to fracture and dislocation nucleation models for SiC



D. Warner (CORNELL U.)



- Activation energy predicted by the continuum model
- Elastic constants(T) + surface energies(T) + unstable stacking fault energies(T) +

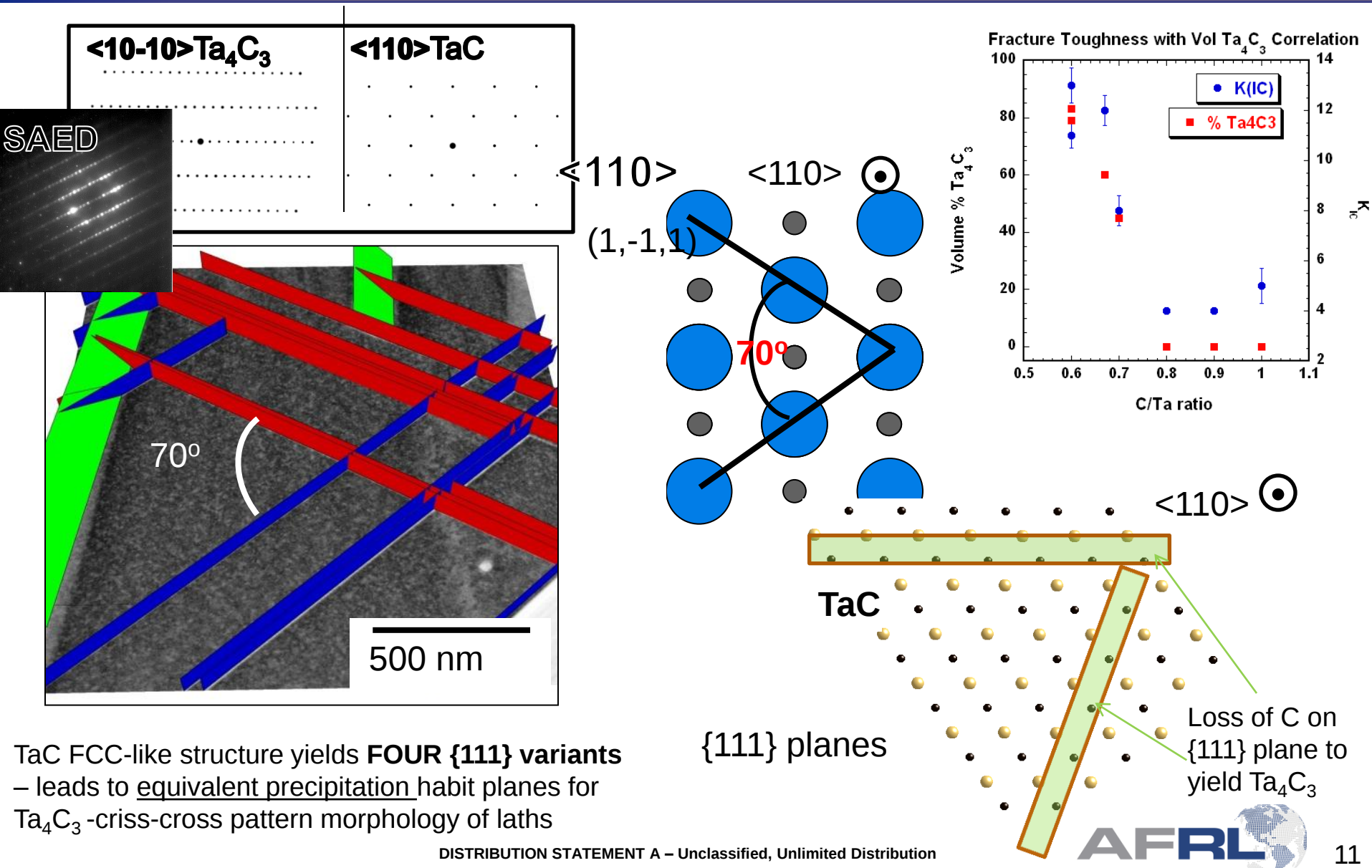
$$\frac{Q_{3D}}{k_B T} = \ln\left(\frac{k_B T N \omega_0}{-\dot{K}_I \frac{dQ_{3D}}{dK_I}}\right)$$



Orientation Relationship of TaC and Ta₄C₃ phase



G. Thompson (U. ALABAMA)

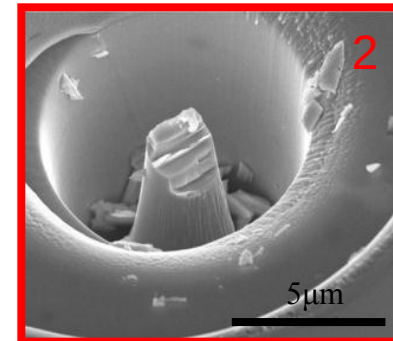
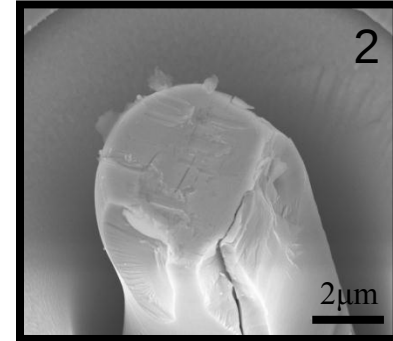
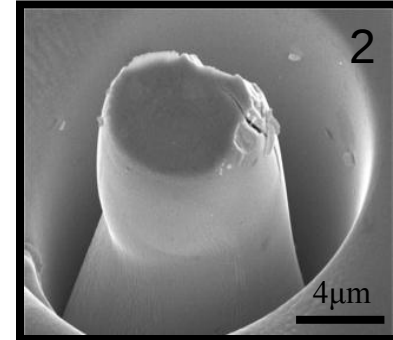
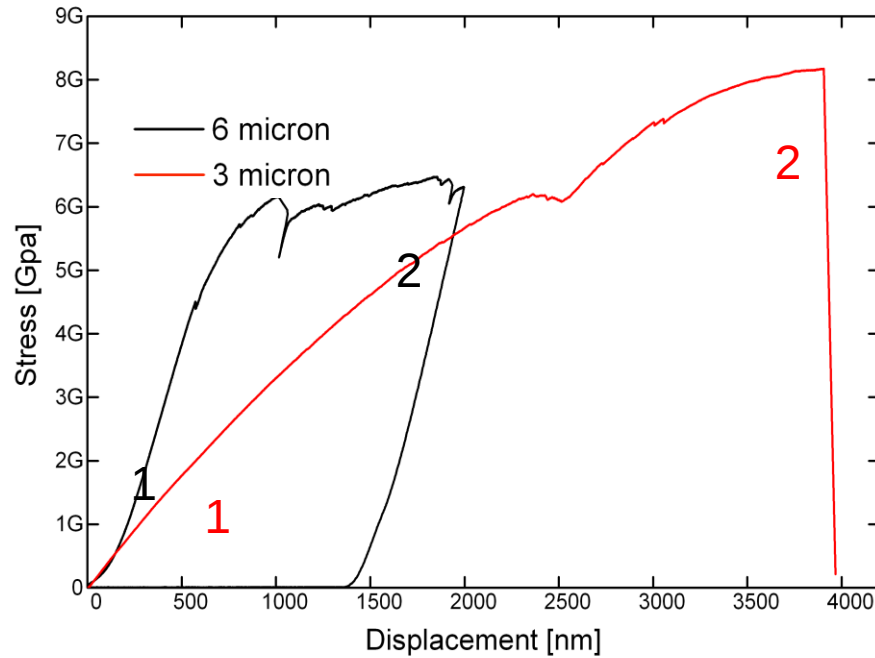
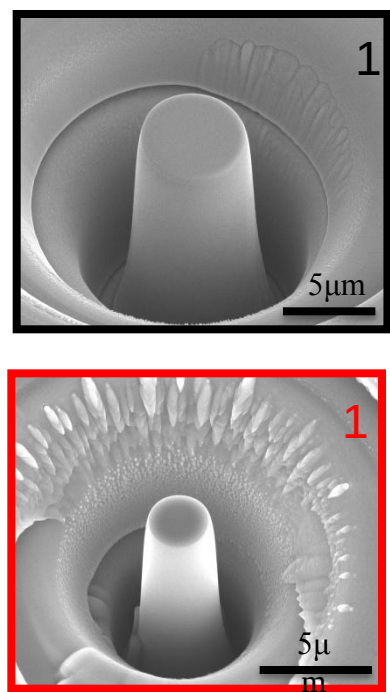




Unsolved Problem: Scale Effect ZrC(001)



S. Kodambaka (UCLA)



- Deviation from linearity
- Pop-in or displacement bursts, buckling, cracking
- Max CRSS on {111} planes
- Plastic flow due to formation of slip bands
- Shearing and cracking rather than catastrophic fracture specially in 6μm pillars



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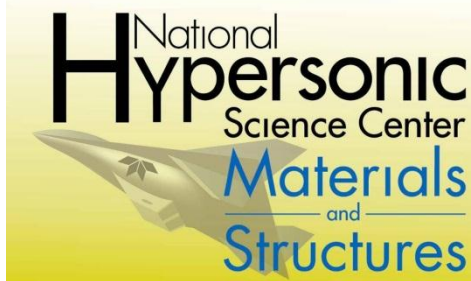
National Hypersonic Science Center



D. Marshall, B. Cox (TELEDYNE), F. Zok (UC SB), B. Fahrenholtz (MST), P. Kroll (UT AUSTIN), Q. YANG (U. MIAMI), R. RITCHIE (UC BERKELEY)

- Highly integrated research program: graduate students & post docs
- 35 journal publications; 23 plenary/keynote presentations at international conferences (including Mueller award lecture at ICACC'12, 4 lectures at 2012 Ceramics Gordon Conference); 12 conference proceedings; 25 other conference papers
- Active collaborations with 10 universities.
- Sharing of data & modeling with AFRL, Army, NASA, Rolls Royce
- Organized International Summer School on Materials for Hypersonics, UCSB, Aug. 2011. Organized International workshop on high-temperature ceramic composites, Boulder CO June 12-15 2012; www.engineceramics.org

www.nhsc-ms.org

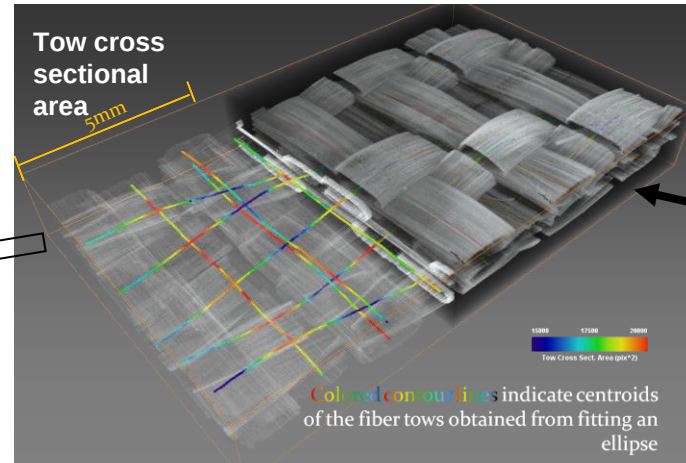




3-D Microstructural Characterization and Geometry Generator

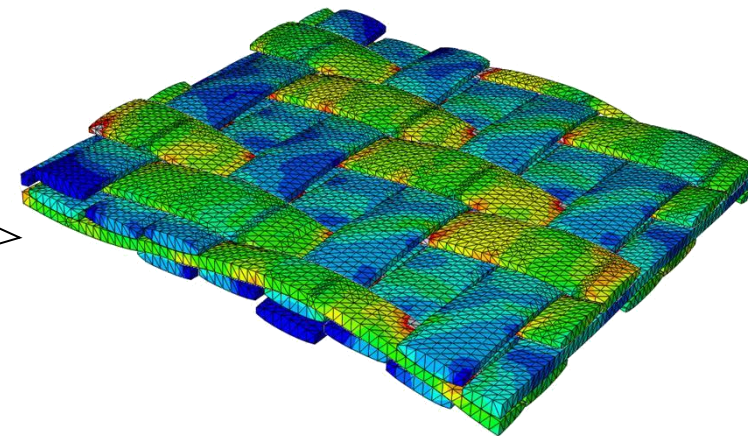
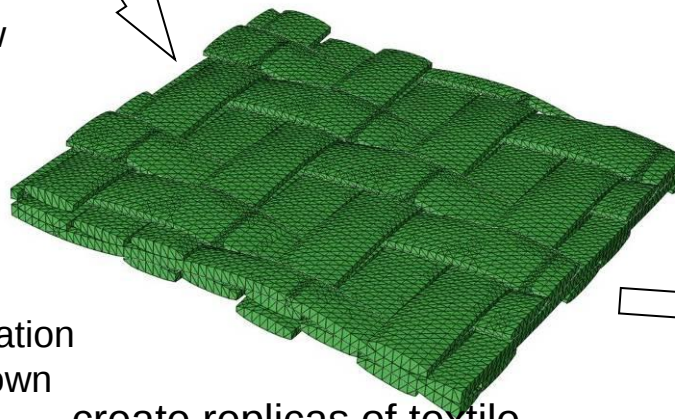


D. Marshall, B. Cox (TELEDYNE), F. Zok (UC SB), Q. YANG (U. MIAMI), R. RITCHIE (UC BERKELEY)



3-D image of C-SiC composite

computational mesh from geometric model



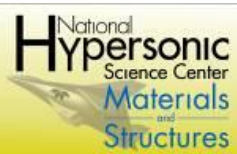
create replicas of textile reinforcement with same statistics as those measured

Statistical description of geometry

Tow paths
Cross-sectional areas
Orientation of cross section
Deviations from mean
Correlation lengths

analogue of Markov chain method for tow axis coordinates $\Rightarrow$ stochastic irregular elliptical cylinder for each tow

problem: interpenetration
solution: enforce known topology of textile



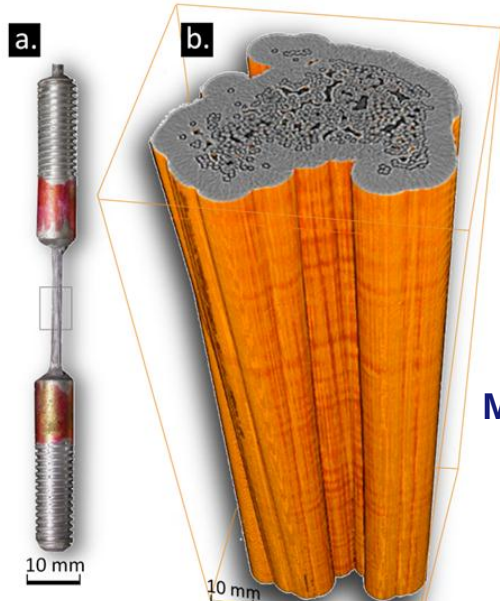


In-Situ 3D Tomography at 1750 c



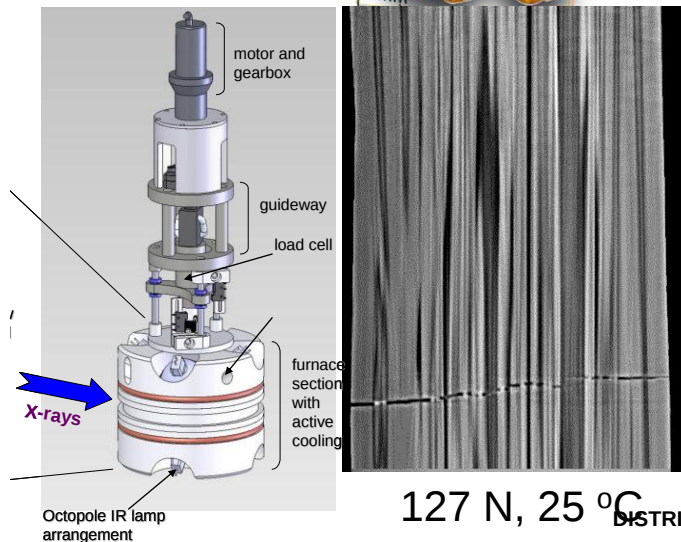
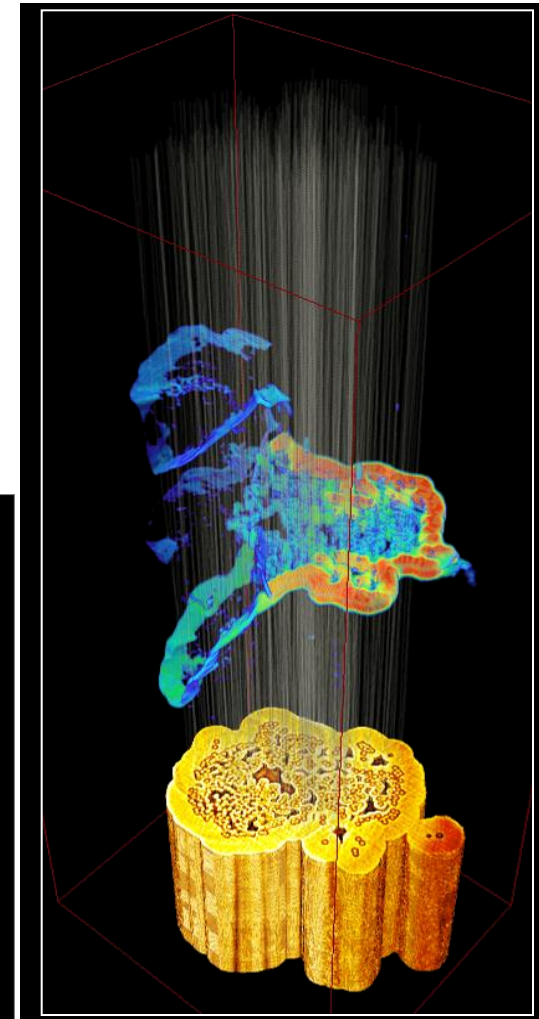
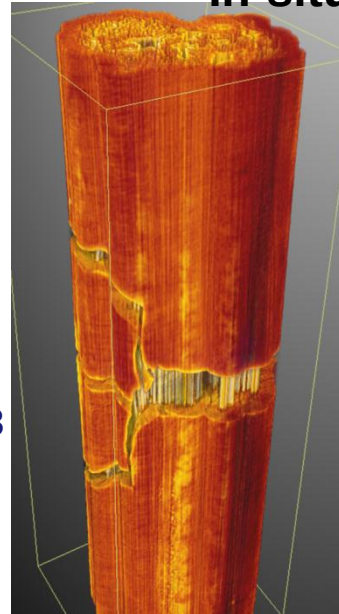
R. Ritchie (UC BERKELEY)

In-situ testing $\text{SiC}_f/\text{SiC}_m$ at 25°C

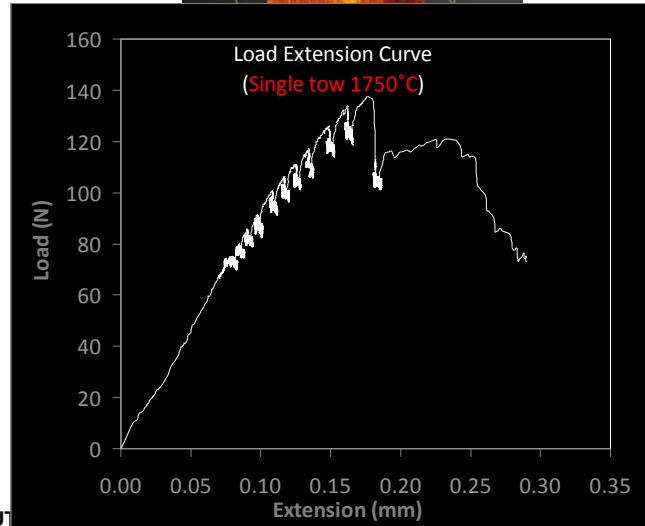


Nature of
Materials 2013

In-situ testing $\text{SiC}_f/\text{SiC}_m$ at 1750°C



127 N, 25 °C

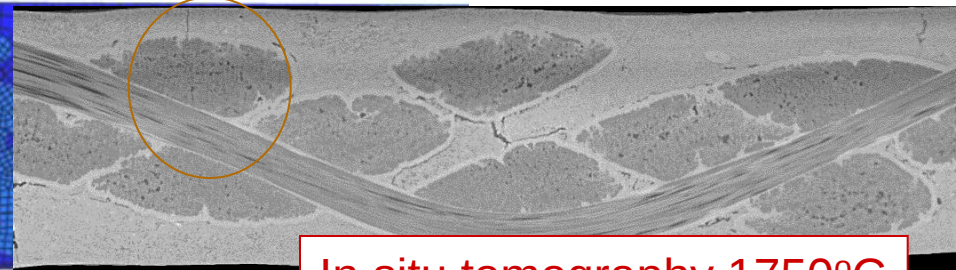
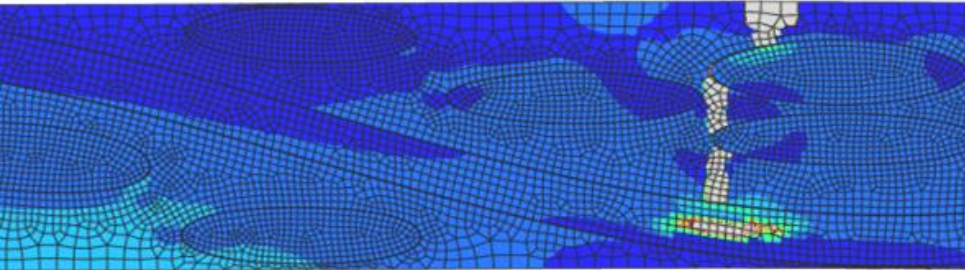




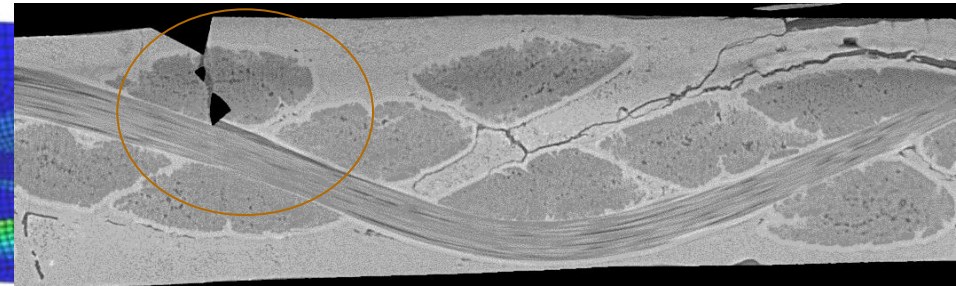
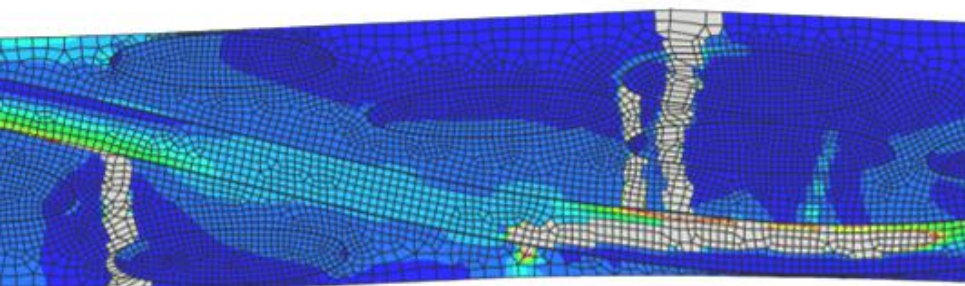
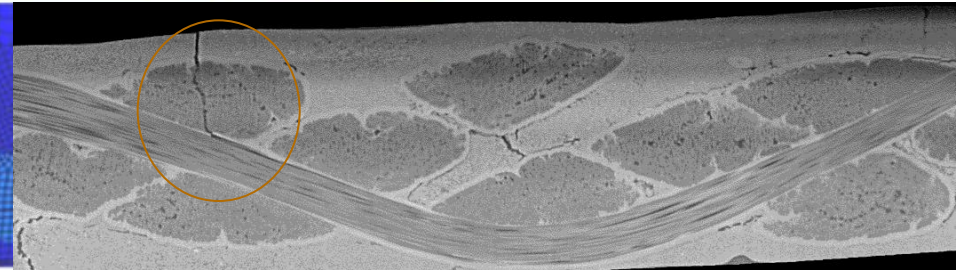
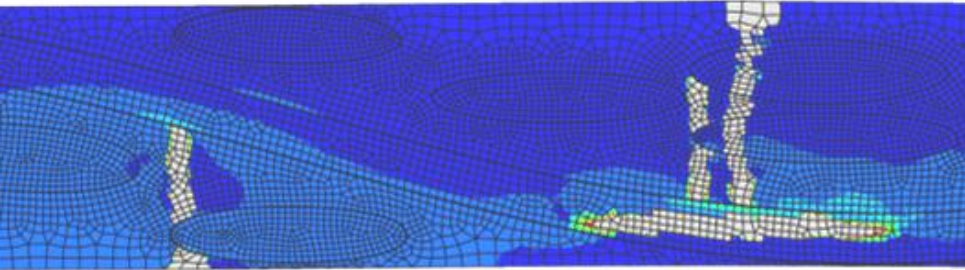
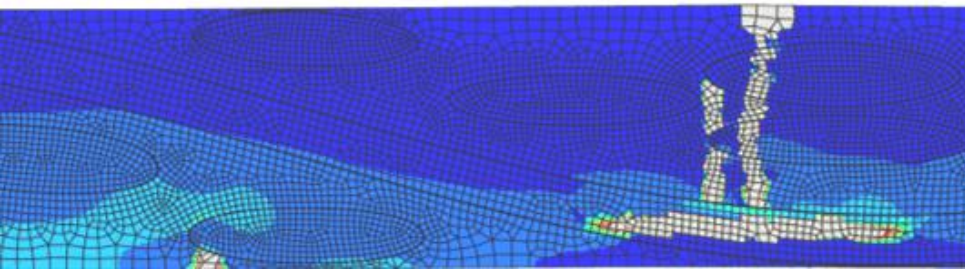
Comparison of Simulation and in-situ Tomography



D. Marshall, B. Cox (TELEDYNE), F. Zok (UCSB), Q. Yang (U. MIAMI), R. Ritchie (UC BERKELEY)



In situ tomography 1750°C





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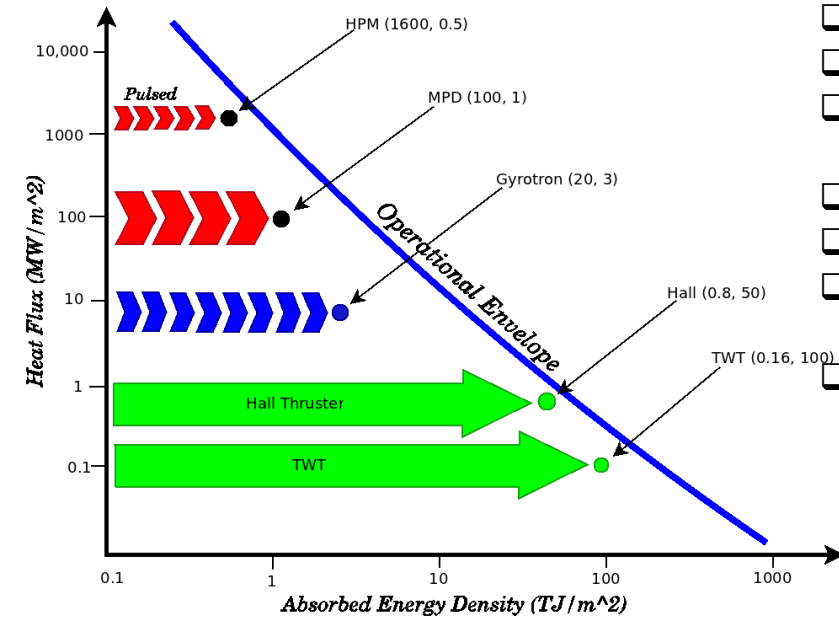
Surface Catalysis at Extreme Environment

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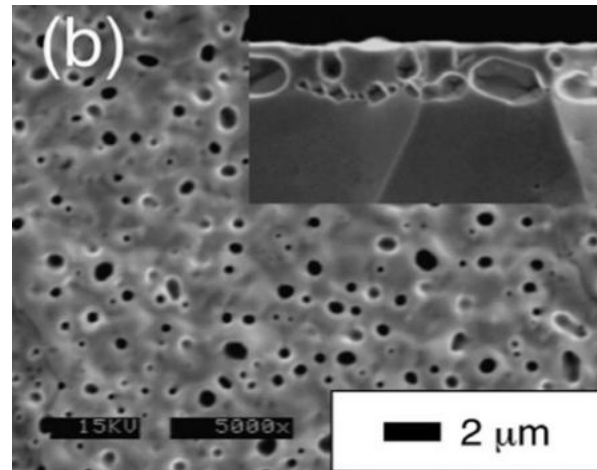
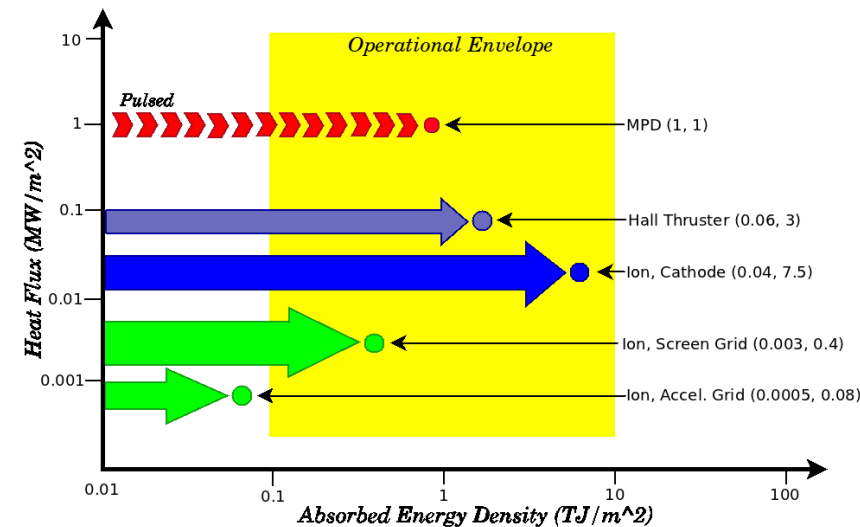


Materials Far from Equilibrium: Micro-Architected Surfaces

N. Ghoniem / UCLA



- ☐ Plasma Erosion & Modeling (Wirz - UCLA).
- ☐ Plasma Source Development (Goebel - JPL/UCLA)
- ☐ Secondary Electron Emission & Plasma Modeling (Raites, Kaganovich - PPPL).
- ☐ Materials Characterization (Thompson - UA).
- ☐ High Heat Flux Testing (Ghoniem - UCLA).
- ☐ Manufacturing of Micro-architected Materials (Williams - ULTRAMET).
- ☐ Multiscale Modeling of Material Damage (Ghoniem - UCLA).



Hole formation
[1994(MJ/m^2),
0.2 (MW/m^2)]



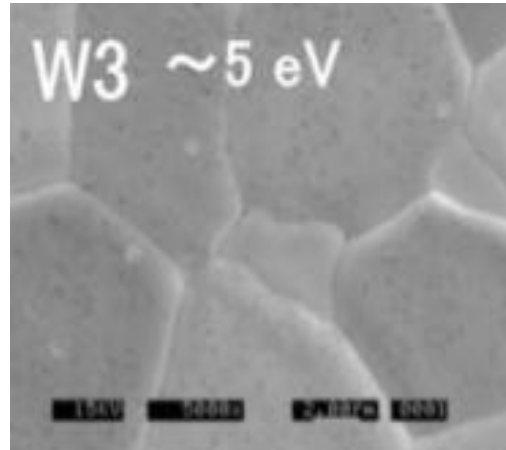
Damage for Heat flux $< 1 \text{ MW/m}^2$



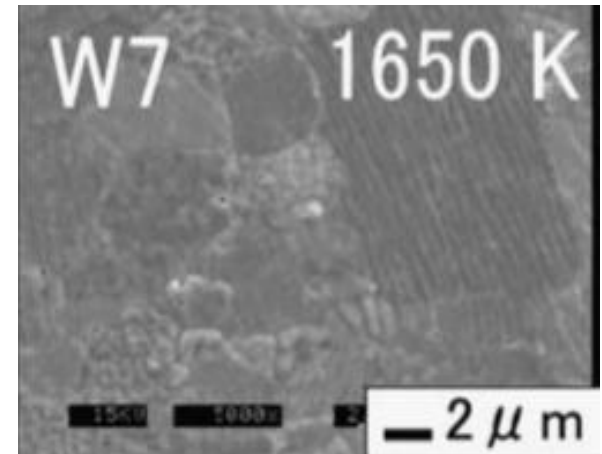
N. Ghoniem (UCLA), Y. Raitses and I. Kaganovich (PRINCETON),
G. Thompson (U. ALABAMA), B. Williams (ULTRAMET)



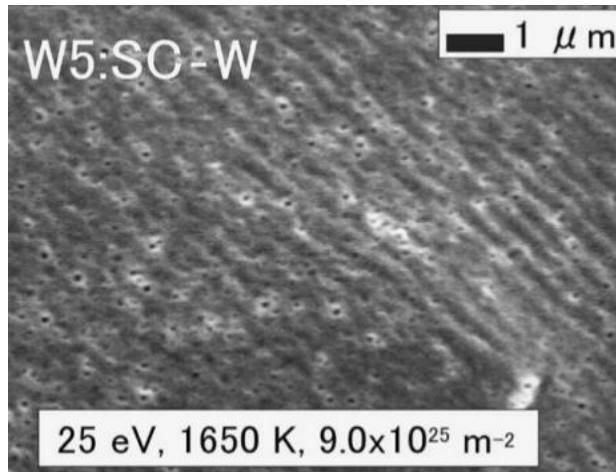
No damage
[128(MJ/m²), 0.02 (MW/m²)]



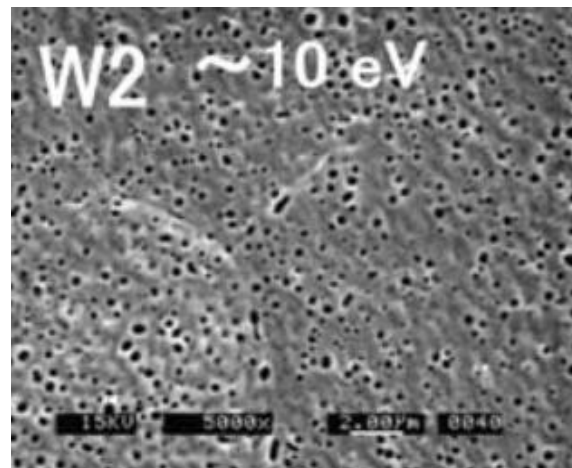
Fine hole formation
[641(MJ/m²), 0.2 (MW/m²)]



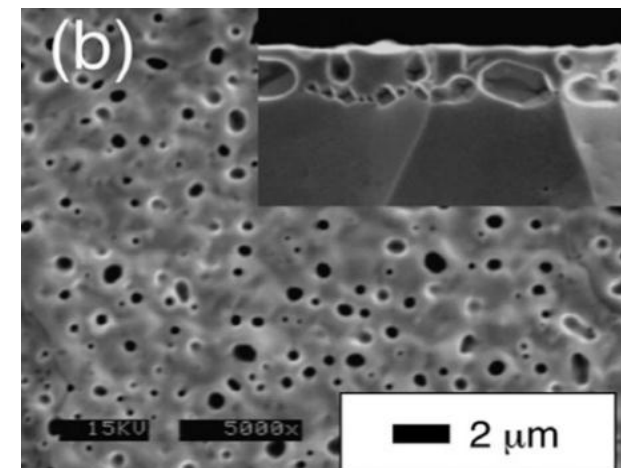
Limited damage
[721(MJ/m²), 0.4 (MW/m²)]



Hole formation
[360 (MJ/m²), 0.2 (MW/m²)]



Hole formation
[1441(MJ/m²), 0.2 (MW/m²)]

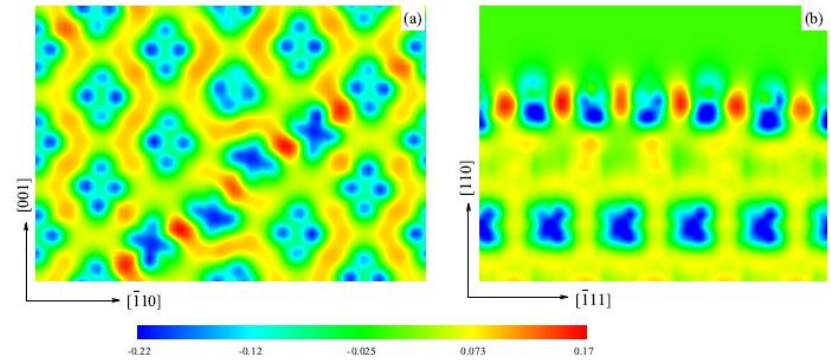
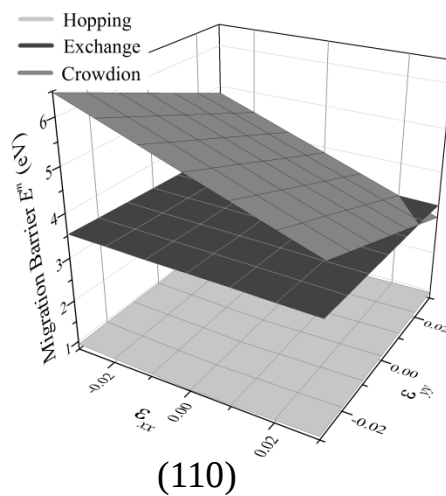
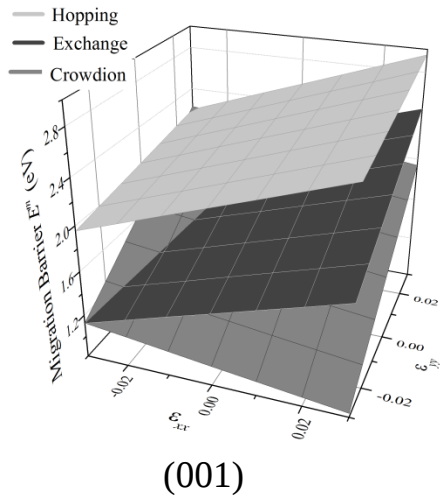


Hole formation
[1994(MJ/m²), 0.2 (MW/m²)]



Atomistic Simulations of Surface Defects in W under Plasma Bombardment

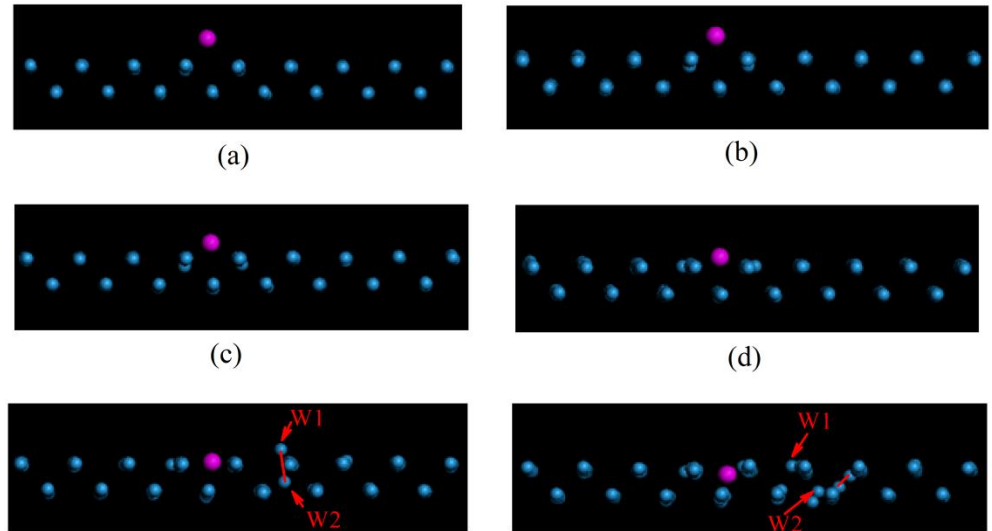
N. Ghoniem (UCLA)



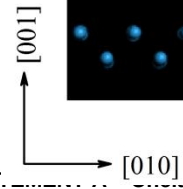
$\rho(r)$ of surface crowdion indicates the high mobility and strong anisotropy of its movement.

Hopping of the adatom is the dominant mechanism on (110) surface. The formation and the movement of surface crowdions contributes mostly on (001) surface. Exchange mechanism is also important on (001) surface, biaxial strain can manipulate the relative contribution of Path-Ex and Path-Crow.

MD simulation indicates that the bombardment of a Xe atom induces ballistic diffusion of W atoms (W1 in the graph) and causes the formation and evolution of crowdions near the surface.



DISTRIBUTION STA:



Snapshots of the bombardment of a Xe atom (KE = 100 eV) on W(001) surface at $T = 200$ K.



Vacancy Production in Surface Layers Leads to Surface Instabilities

N. Ghoniem (UCLA)

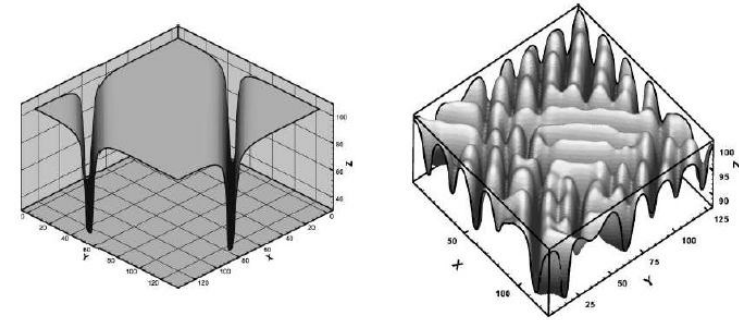
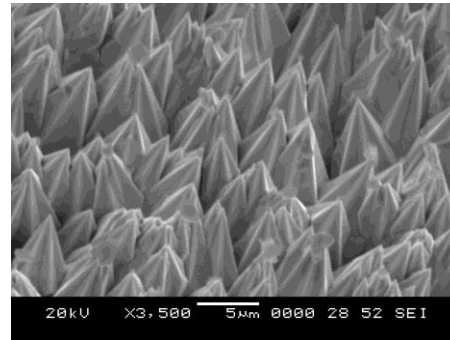
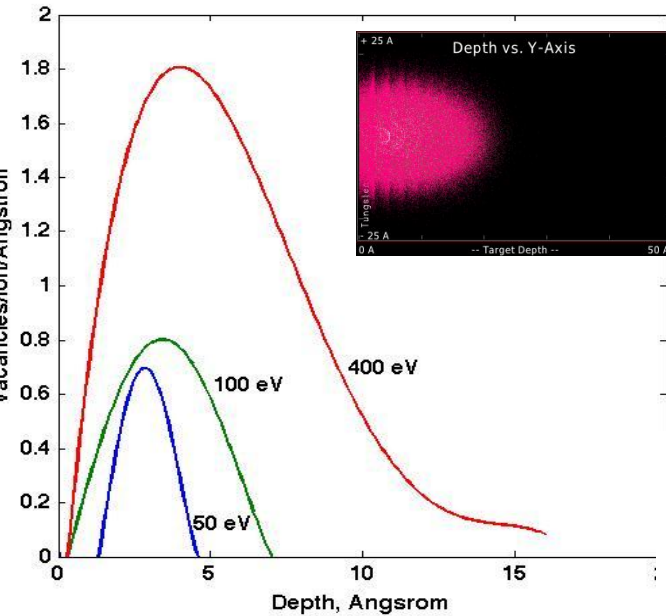
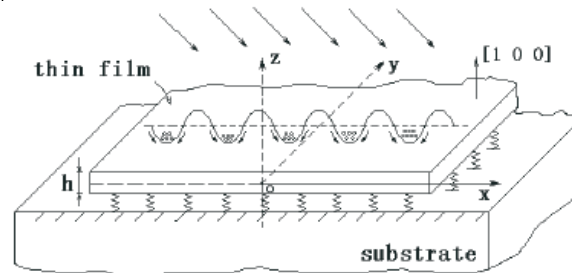


FIG. 14.20. Groove patterns seen under a biaxial stress state in which one side is under tension and the other is under compression [713].



D. Walgraef, N.M. Ghoniem, and J. Lauzeral. Deformation patterns in thin films under uniform laser irradiation. *Phys.Rev., B* 56:15361–15377, 1997.

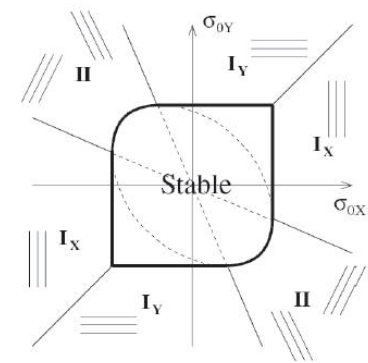


FIG. 14.21. Pattern selection in biaxial laser irradiation [713].

$$\nabla \cdot \mathbf{U} = -zm\Delta\xi,$$

$$\partial_t^2 \xi + \frac{c^2 h^2}{12} \Delta^2 \xi - \frac{c^2}{2} \sigma_{ij} \partial_{ij}^2 \xi + \frac{\theta_v}{\rho h} (C_+ - C_-) = 0, \quad \partial_t C = D_{\perp} \partial_{zz}^2 C + D_{\parallel} \Delta C - \frac{C}{\tau} + \nabla \frac{\theta_v D_{\parallel} C}{kT} \nabla (\nabla \cdot \mathbf{U})$$

$$+ \nabla_z \frac{\theta_v D_{\perp} C}{kT} \nabla_z (\nabla \cdot \mathbf{U}) + g \exp\left[-\frac{E_f}{kT}\right] (1 + \theta_v \nabla \cdot \mathbf{U})$$

Jerome Paret. Long-time dynamics of the three-dimensional biaxial grinfeld instability. *Physical Review E*, 72:01105–1–5, 2005.



OUTLINE



I. Predictive Materials Science

Bulk Metallic Glasses

Carbides (SiC, TaC, Ta₄C)

Textile Based Hybrid Composite

II. Materials Far from Equilibrium

Micro-Architected Surfaces

Surface Catalysis at Extreme Environment

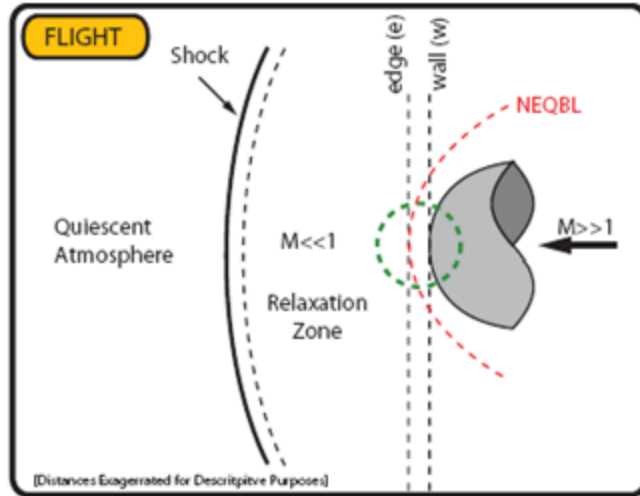
III. Challenges, Motivations and New initiatives.



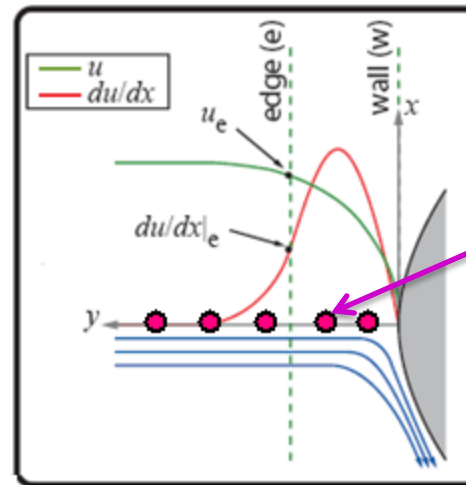
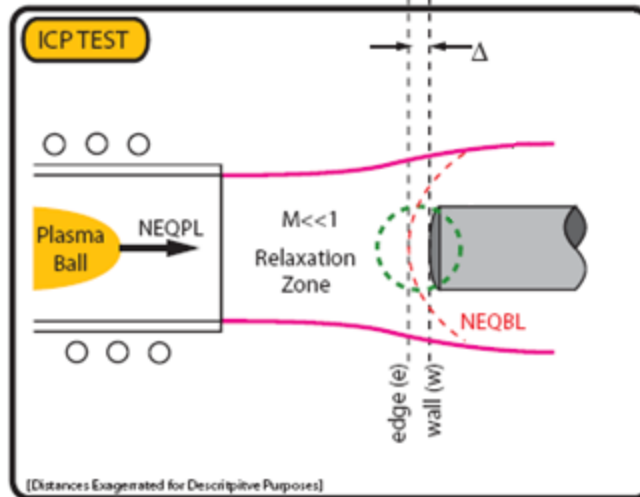
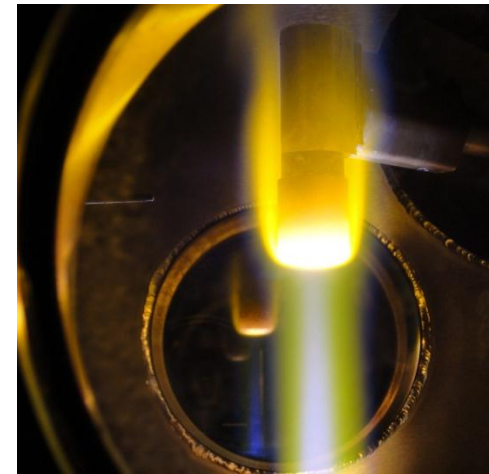
Surface Catalysis Testing in a 30kW ICP Torch Facility



D. Fletcher (U. VERMONT), J. Marshall (SRI), M. Akinc (ISU), J. Prepezko (U. Wisconsin)



Approach: Compare surface-catalyzed reaction efficiencies for flexible and rigid materials with same elemental composition by measuring relative atom density and temperature gradients above material samples in the 30 kW ICP Torch Facility using laser induced fluorescence



Spatially resolved measurement location

Flight environment to ground facility testing comparison

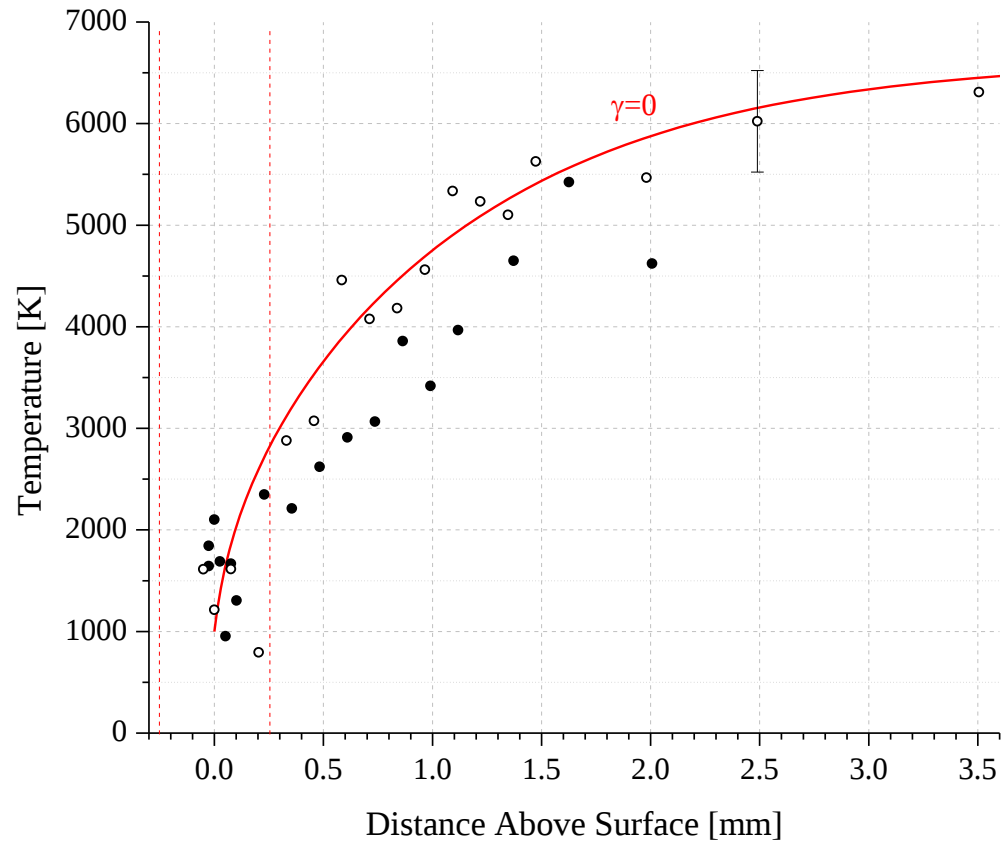
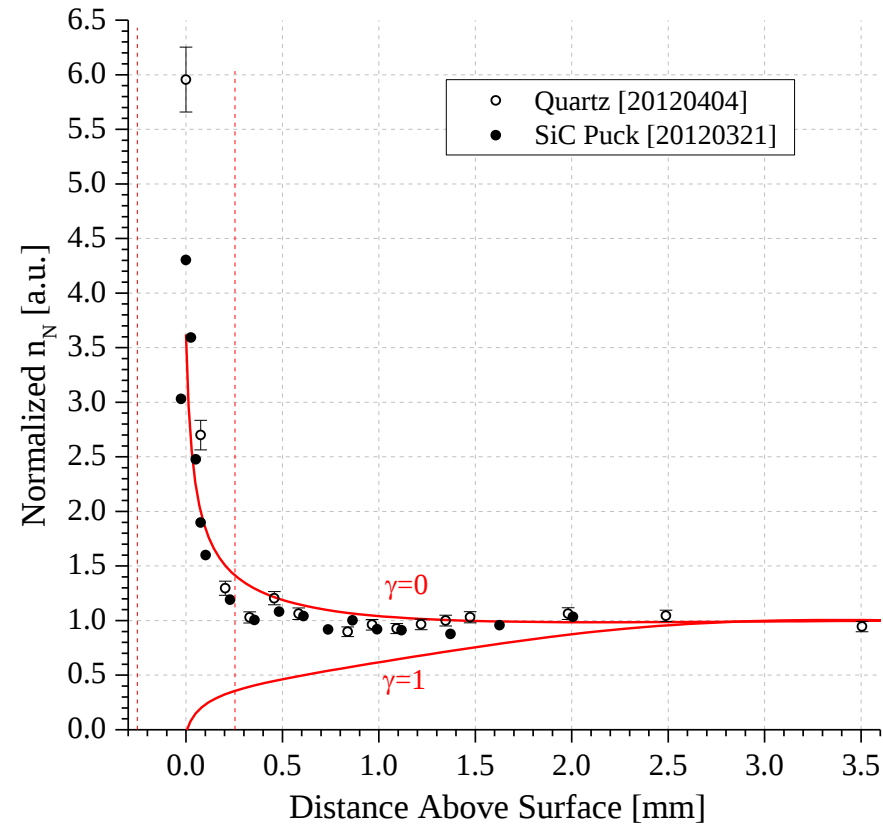




Surface Catalytic Effect of SiC Testing in a 30kW ICP Torch Facility



D. Fletcher (U. VERMONT), J. Marshall (SRI), M. Akinc (ISU), J. Prepezko (U. Wisconsin)



- Relative N atom concentration measurements for quartz and monolithic α -SiC
- Increasing concentration toward wall indicates low surface catalyzed reaction efficiency
- From the n_N plot, it can be seen that α -SiC ($T_w = 1300$ K) is of comparable catalycity to quartz ($T_w < 1000$ K)



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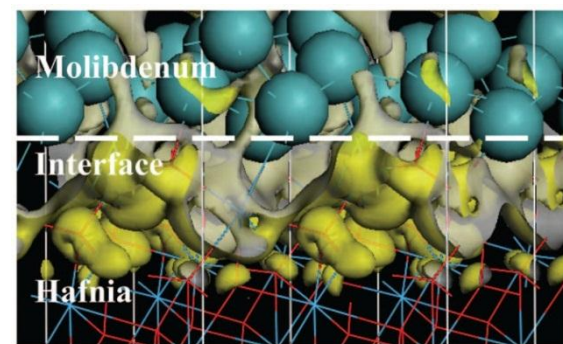
Surface Catalysis at Extreme Environment

III. Challenges, Motivations and New initiatives.

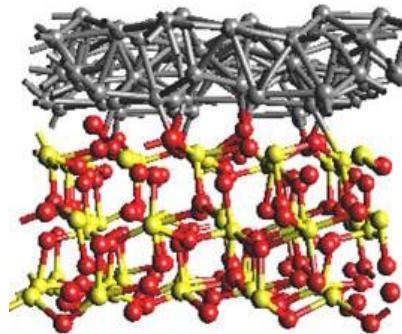


2012 BRI: 2D-Materials for Extreme Environments

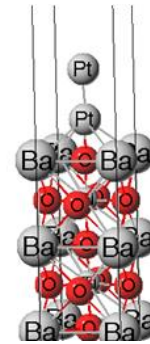
2013 BRI: Charge Transfer at the Interface



Demkov 2010



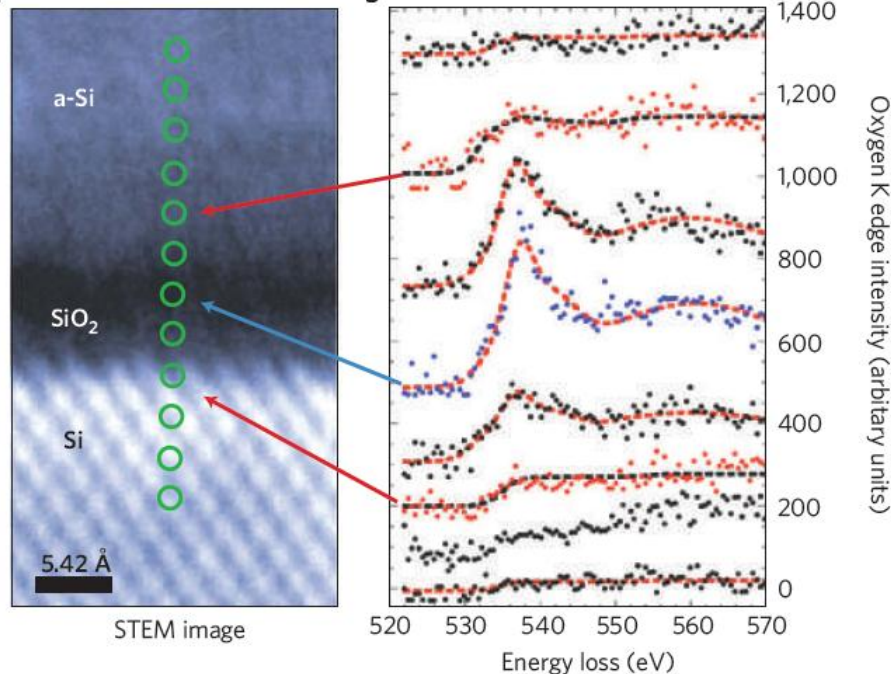
Inoue 2009



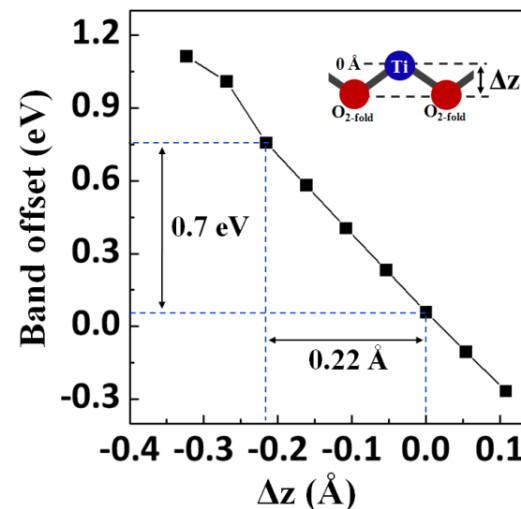
Heidger 2012

- Demkov: Diffuse Interface
- Inoue: Stoichiometry of $\text{Hf}_{1-x}\text{O}_{2-\xi}$
- Heidger: Termination

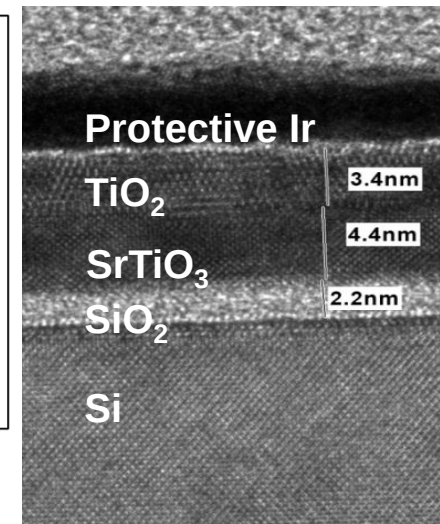
Electron Energy Loss Spectroscopy



Interfacial dielectric response



A. Demkov, unpublished work





SUMMARY



I. Predictive Materials Science

Bulk Metallic Glasses

Carbides (SiC, TaC, Ta₄C)

Textile Based Hybrid Composite (NHSC)

2012 MURI: Mosaic of Structure (CMU): Descriptor Challenge (wt. Dr. Fahroo)

2012 MURI: Atomic Scale Interface (LEHIGH) / (Dr. Shifler / ONR)

2013 MURI: Peridynamics (wt. Drs. Stargel & Fahroo)

II. Materials Far from Equilibrium

Micro-Architected Surfaces

Surface Catalysis at Extreme Environments

2013 BRI: Layered Structured Materials (2D E-Gas)

III. Challenges, Motivations and New initiatives

2012 MURI: Template-Directed Directionally Solidified Eutectic Metamaterials

2013 MURI: Magneto-Electric Energy Conversion Materials and Terahertz Emission in Unbiased Dielectrics (wt. Dr. Luginsland)

2013 BRI: Metal Dielectric Interface: Charge Transfer in Heterogeneous Media under Extreme Environments (wt. Dr. Luginsland)