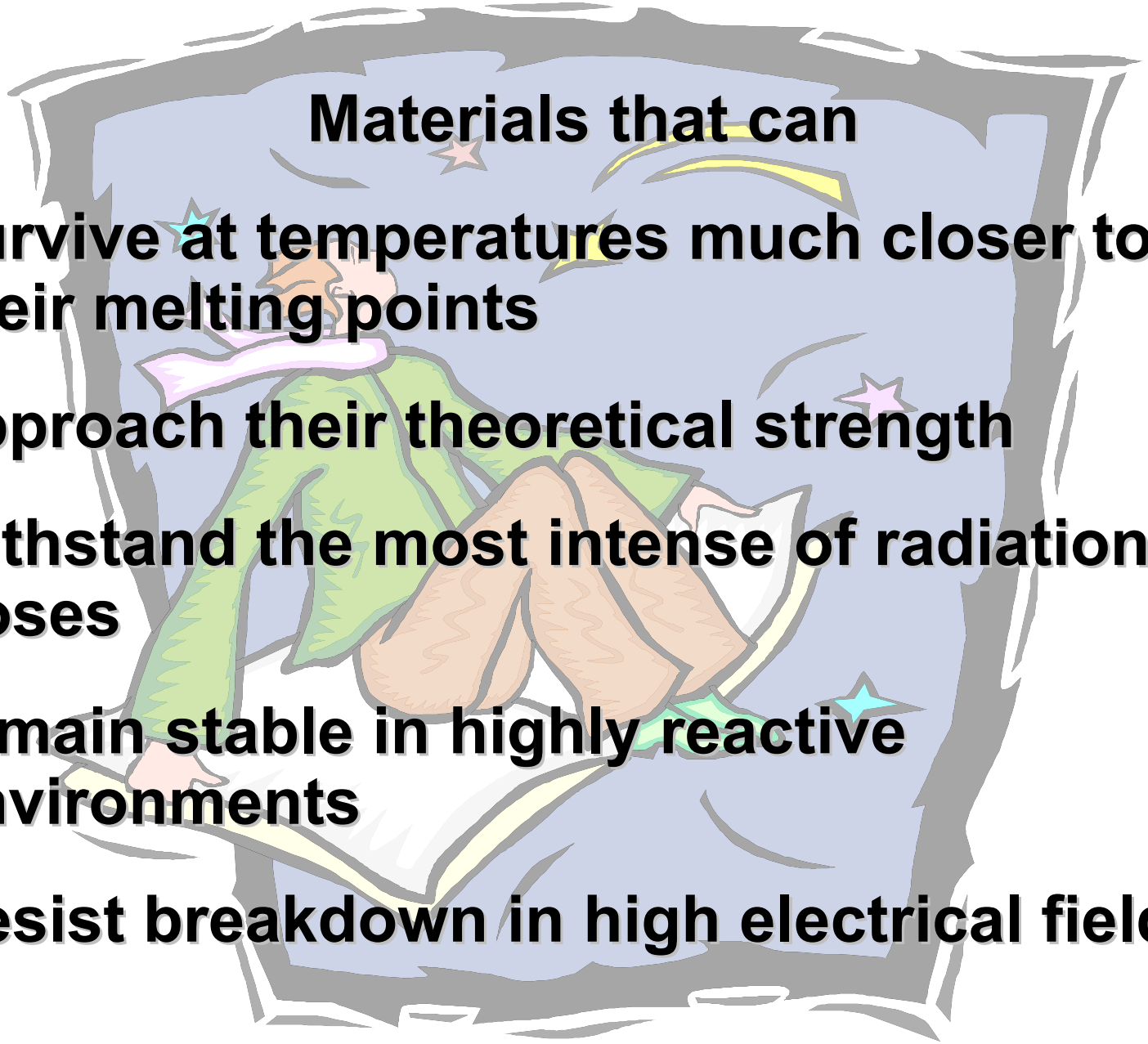
Just Imagine!

Oak Ridge National Laboratory

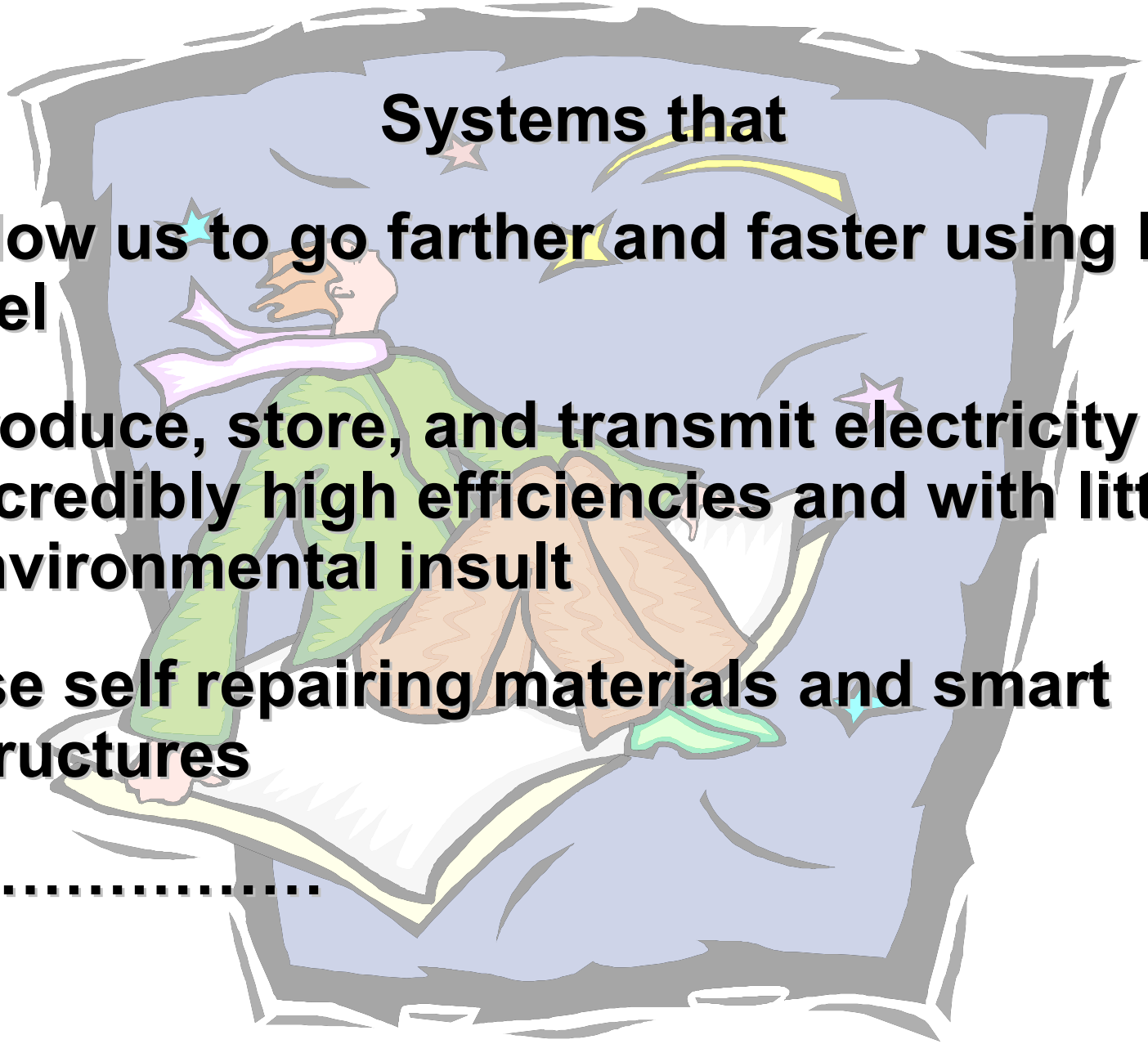
Just Imagine



Materials that can

- survive at temperatures much closer to their melting points
- approach their theoretical strength
- withstand the most intense of radiation doses
- remain stable in highly reactive environments
- resist breakdown in high electrical fields

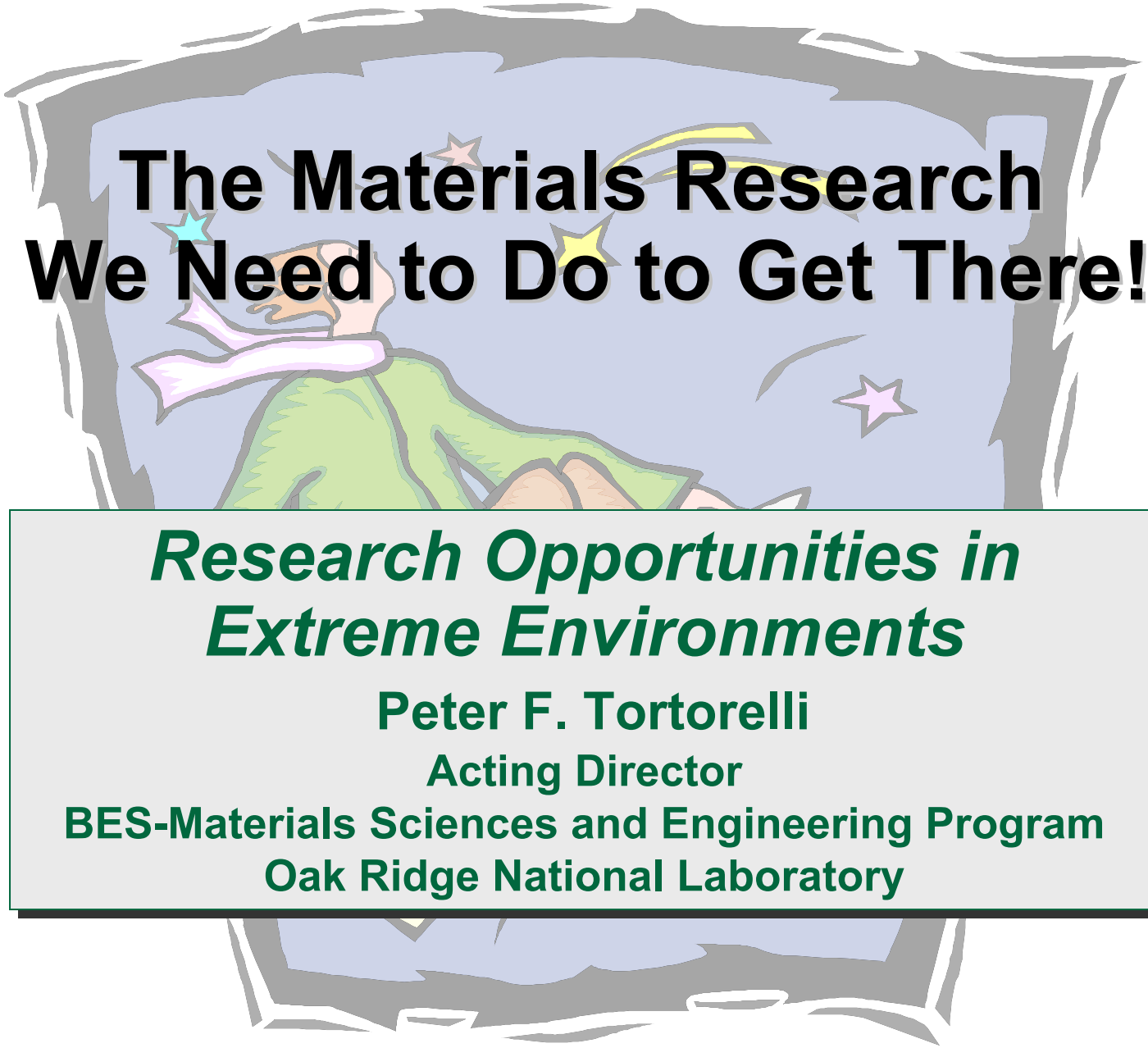
Just Imagine



Systems that

- allow us to go farther and faster using less fuel
- produce, store, and transmit electricity at incredibly high efficiencies and with little environmental insult
- use self repairing materials and smart structures
- ……

Just Imagine



The Materials Research We Need to Do to Get There!!

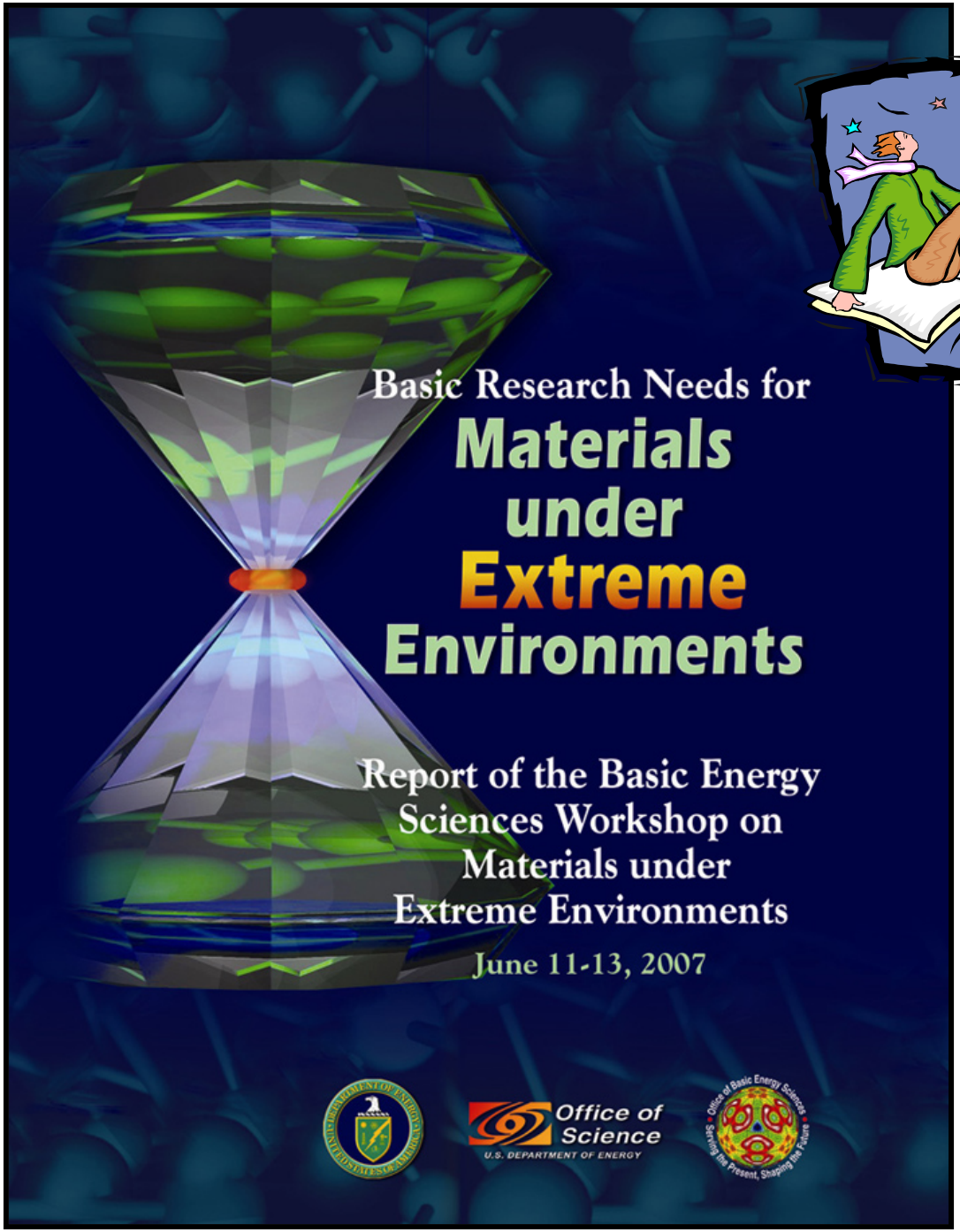
Research Opportunities in Extreme Environments

Peter F. Tortorelli

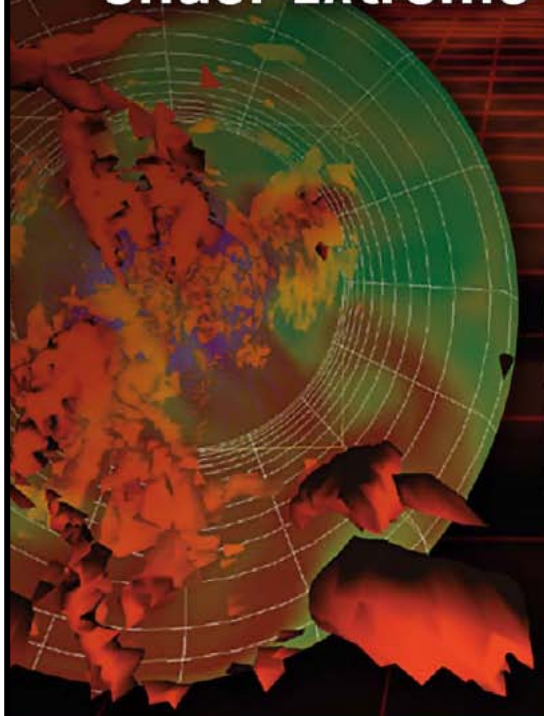
Acting Director

BES-Materials Sciences and Engineering Program

Oak Ridge National Laboratory


Basic Research Needs for
Materials under Extreme Environments
Report of the Basic Energy Sciences Workshop on Materials under Extreme Environments
June 11-13, 2007
Office of Science
U.S. DEPARTMENT OF ENERGY

Technology and Applied R&D Needs for Materials Under Extreme Environments



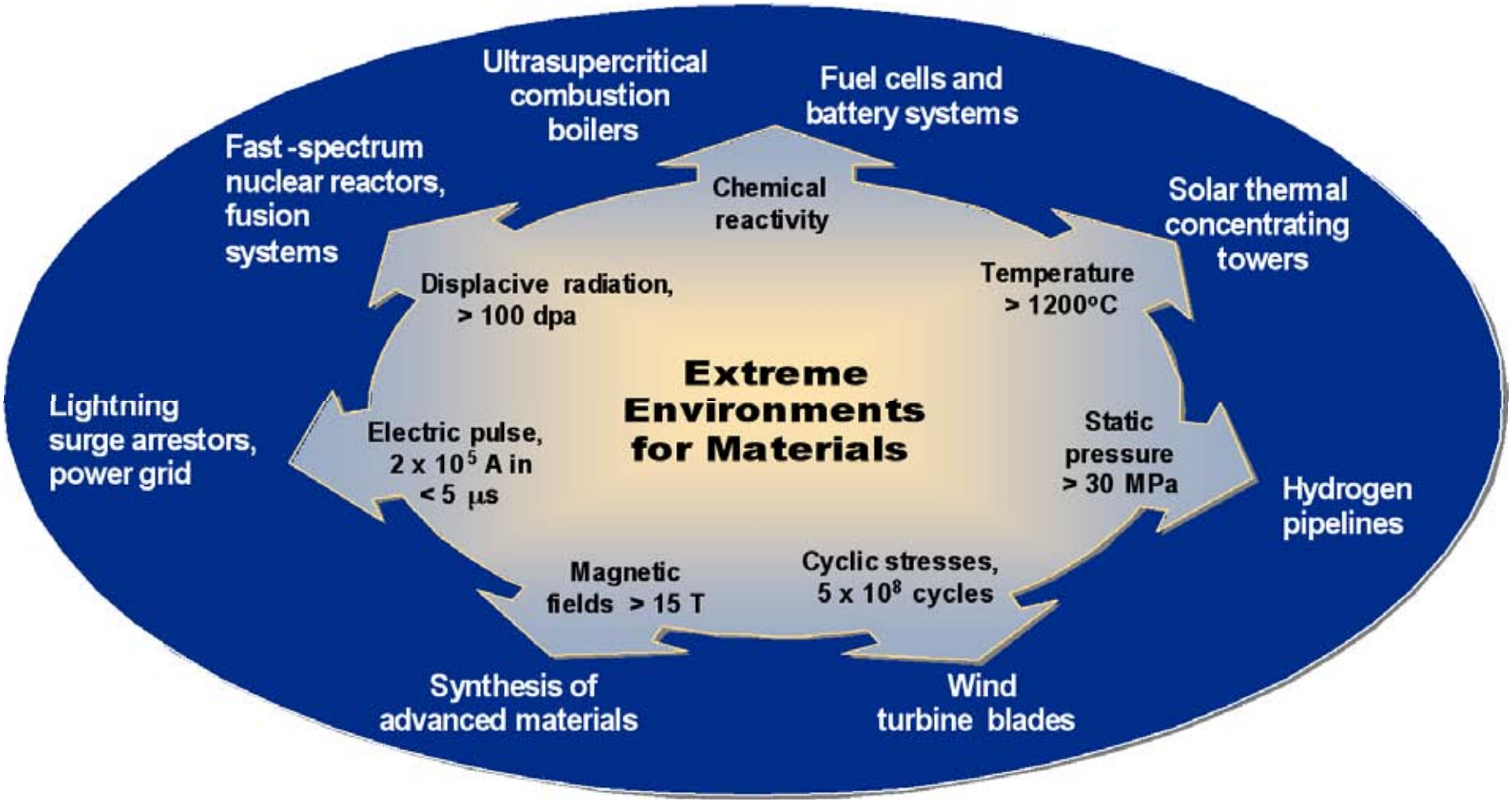
Resource Document for the Workshop on Basic Research Needs for Materials Under Extreme Environments

May 2007

Office of Science
U.S. DEPARTMENT OF ENERGY

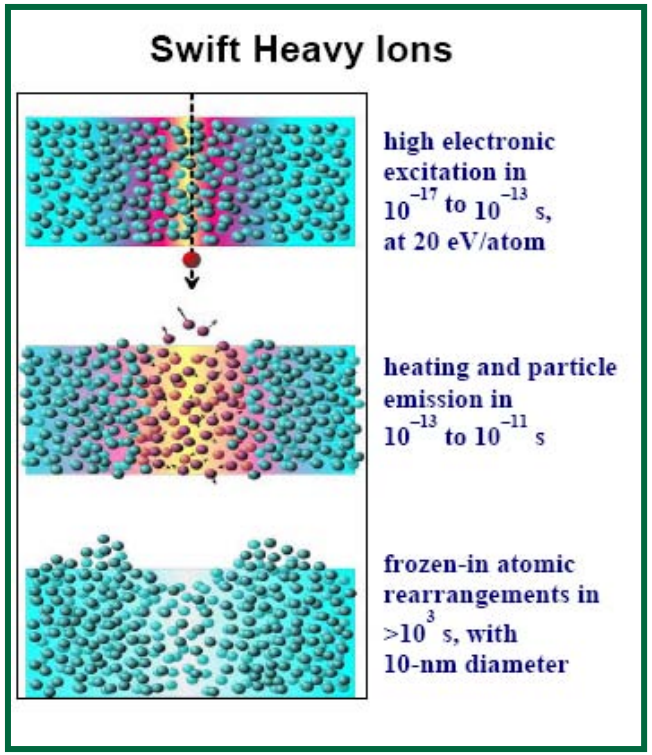
Office of Basic Energy Sciences
Serving the Present, Shaping the Future

Harsh Environments Will Become Extreme With Advances in Many Energy Technologies

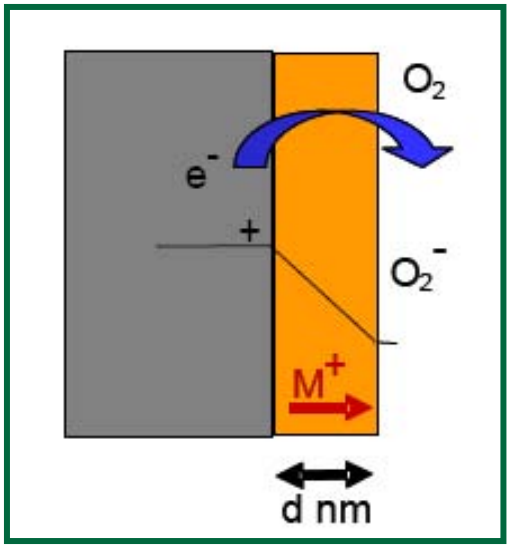


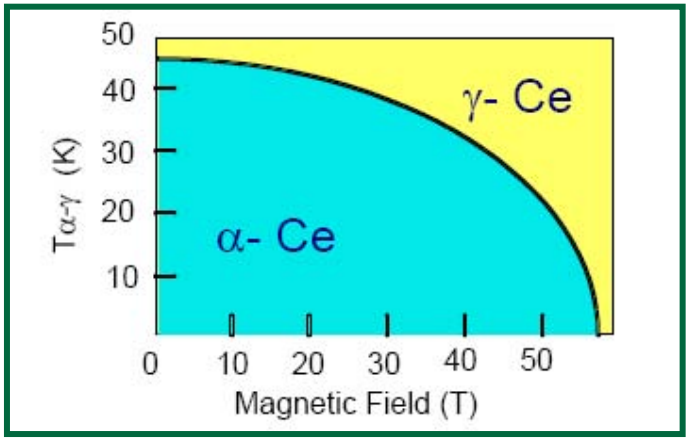
Basic Research Needs for Materials under Extreme Environments, 2007

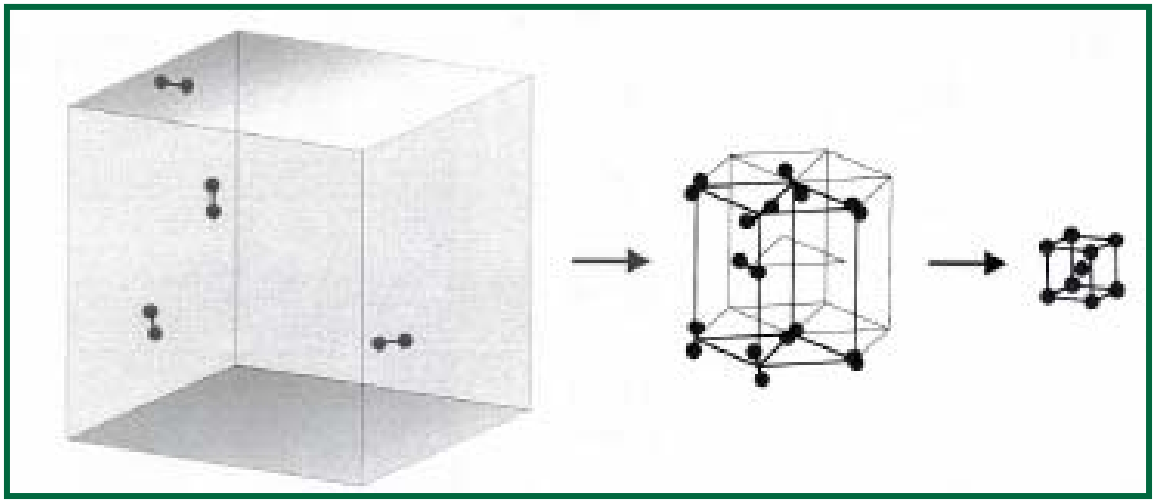
Four Extremes Panels Were Convened (Plus Crosscutting)



- Energetic Flux
- Chemical
- Thermomechanical
- Electromagnetic

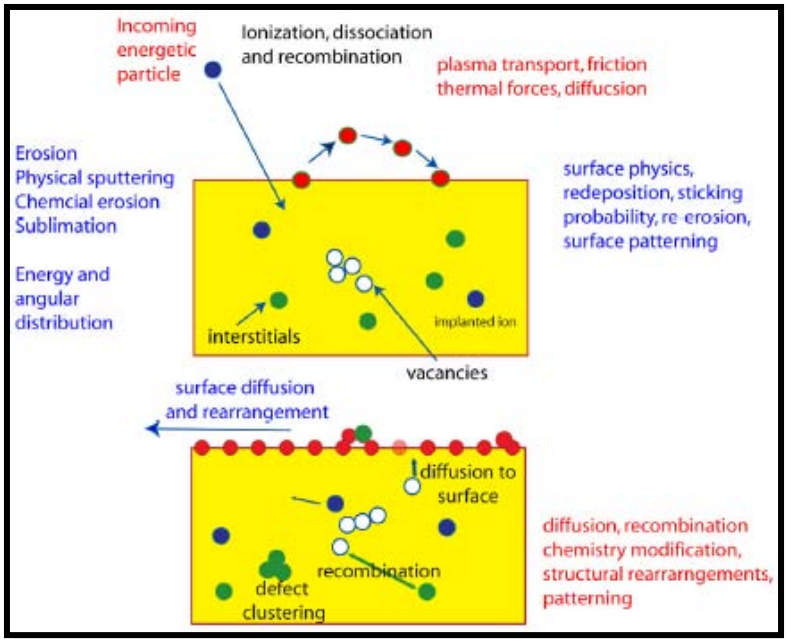






Discussions Revolved Around Key Scientific Questions

- How are processes that are typically controlled by morphology, structure, and defects affected by extremes?
- How do reaction pathways and mechanisms, and transport change when materials are subjected to either static or dynamic extremes



- What new phenomena emerge? Can these be exploited in a beneficial manner, such as for novel synthesis?
- Can processes that occur at extremes be modeled computationally to predict lifetimes or new/existing materials?
- Can we experimentally probe these phenomena?

Priority Research Directions Were Defined

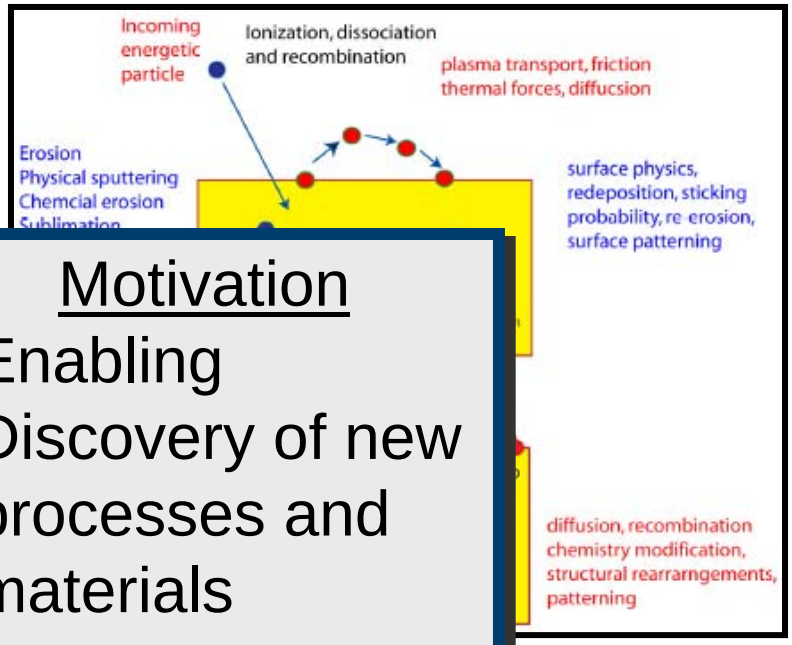
- Design of Materials with Revolutionary Tolerance to Extreme Photon and Particle Fluxes
- Nonequilibrium Synthesis and Processing with Energetic Particle and Photon Beams
- Toward Ideal Surface Stability
- Fundamental Reaction Dynamics at Extremes
- Novel Materials by Design—What is Possible Beyond What We Know
- Disordered, Nanophase, and Composite Materials
- Exploring Thermomechanical Limits of Materials
- High-Performance Electric and Magnetic Materials

"Challenges and Opportunities" Was a Common Reaction Emerging from All Panels

- Challenges
  - Things are hard enough already with respect to understanding performance and lifetime limitations in harsh environments and in designing and selecting materials for such
  - How will we study extreme phenomena?

- Opportunities
  - Potential to open up new regimes of materials behavior that foster discovery
    - New materials
    - Insights into heretofore unexplored reaction pathways and product speciation
    - Next generation materials design/selection paradigms
  - New synthesis methods

There's A Sense of Optimism That We Can Meet the Challenges



- How are processes that are typically controlled by morphology, structure, and defects affected by extreme
- How do reaction pathways and mechanisms, and transport cha when materials are subjected to either static or dynamic extreme
- What new phenomena emerge? Can these be exploited in a beneficial manner, such as for novel synthesis?

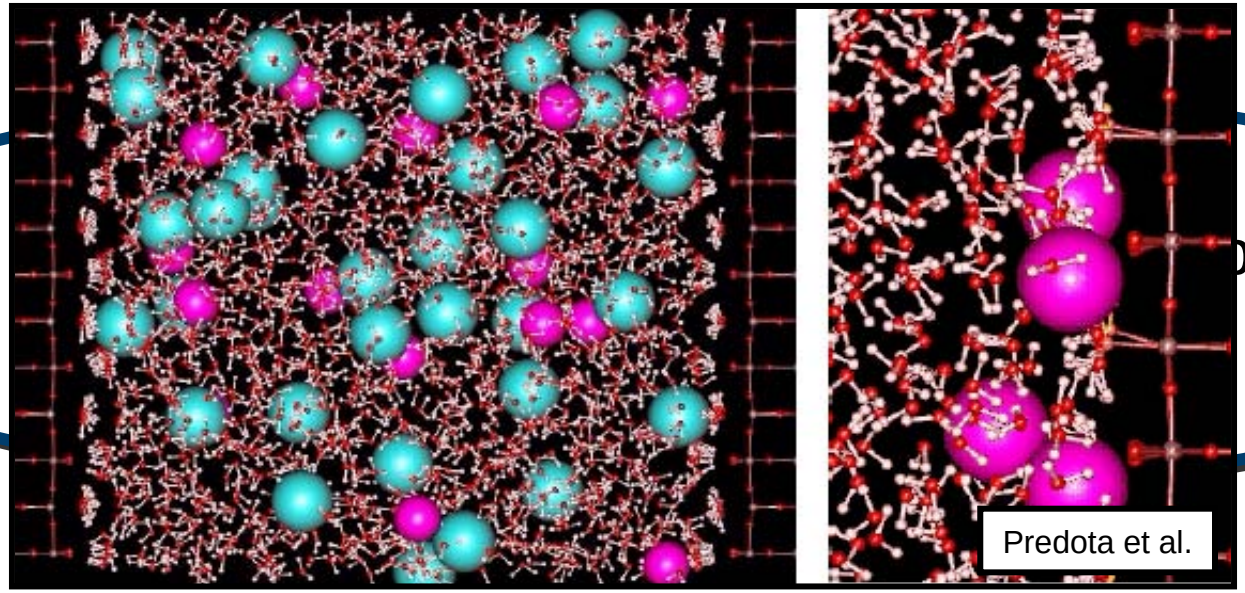
Motivation

- Enabling
- Discovery of new processes and materials

- Can processes that occur at extremes be modeled computationally to predict lifetimes or new/existing materials?
- Can we experimentally probe these phenomena?

Four Recurring Science Issues Emerged

1) Achieving the Limits of Performance
2) Exploiting Extreme Environments for Materials Synthesis and Design
3) Characterizing on the Scale of Fundamental Interactions
4) Predicting and Modeling Materials Performance.



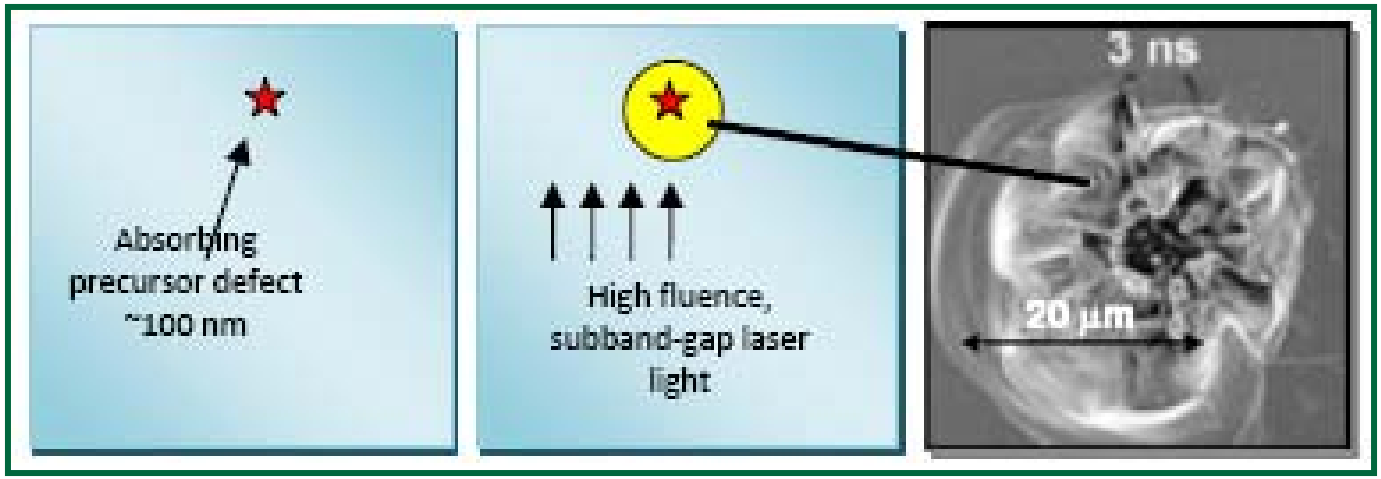
pproaches

Priority Research Directions

- Design of Materials with Revolutionary Tolerance to Extreme Photon and Particle Fluxes **[Perf]**
- Nonequilibrium Synthesis and Processing with Energetic Particle and Photon Beams **[Syn]**
- Toward Ideal Surface Stability **[Perf]**
- Fundamental Reaction Dynamics at Extremes **[Perf, Syn]**
- Novel Materials by Design—What is Possible Beyond What We Know **[Syn]**
- Disordered, Nanophase, and Composite Materials **[Perf, Syn]**
- Exploring Thermomechanical Limits of Materials **[Perf]**
- High-Performance Electric and Magnetic Materials **[Perf, Syn]**

Can Consider Two Extreme Aspects of Performance

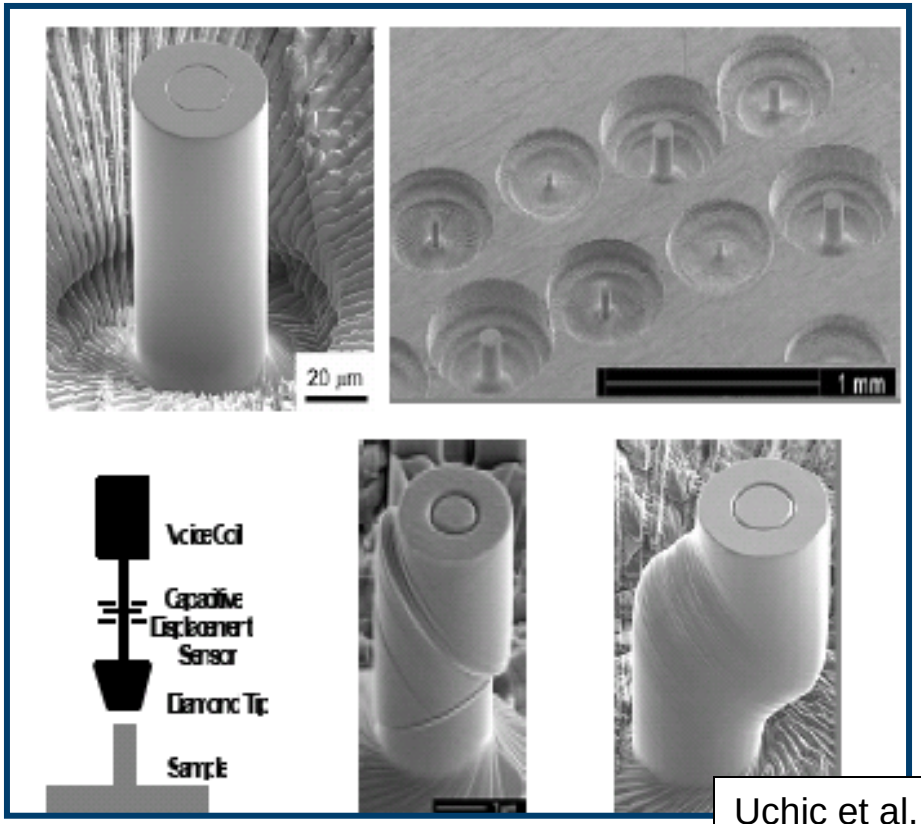
- Resistance to environmental degradation at extremes (e.g., radiation damage, corrosion, dielectric breakdown, etc.)



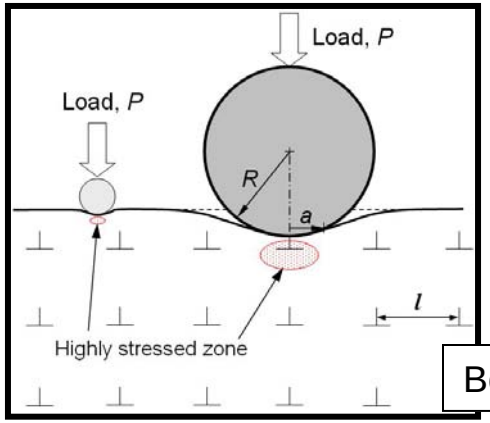
- Reaching theoretical performance, relative extremes (e.g., strength, structural stability, etc.)

Exploring the Ultimate Strength of Materials

- Currently, we typically achieve just a few percent of theoretical strength
- Understanding defects at the atomic and nanoscale, particularly line defects (dislocations) for hard materials
- Emerging new tools and new understanding – hard and soft materials

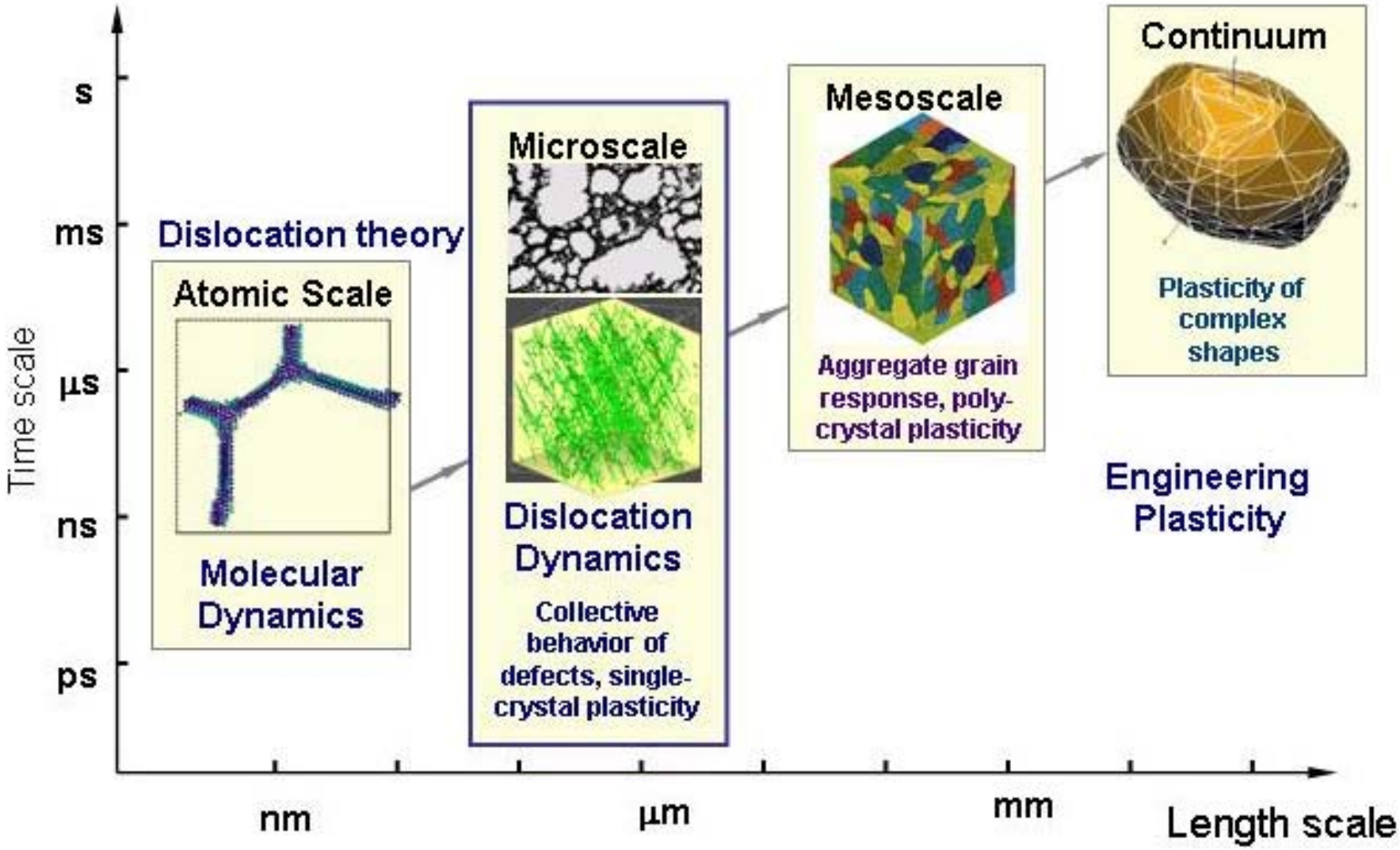


Uchic et al.
Dimiduk et al.
Dimiduk et al.

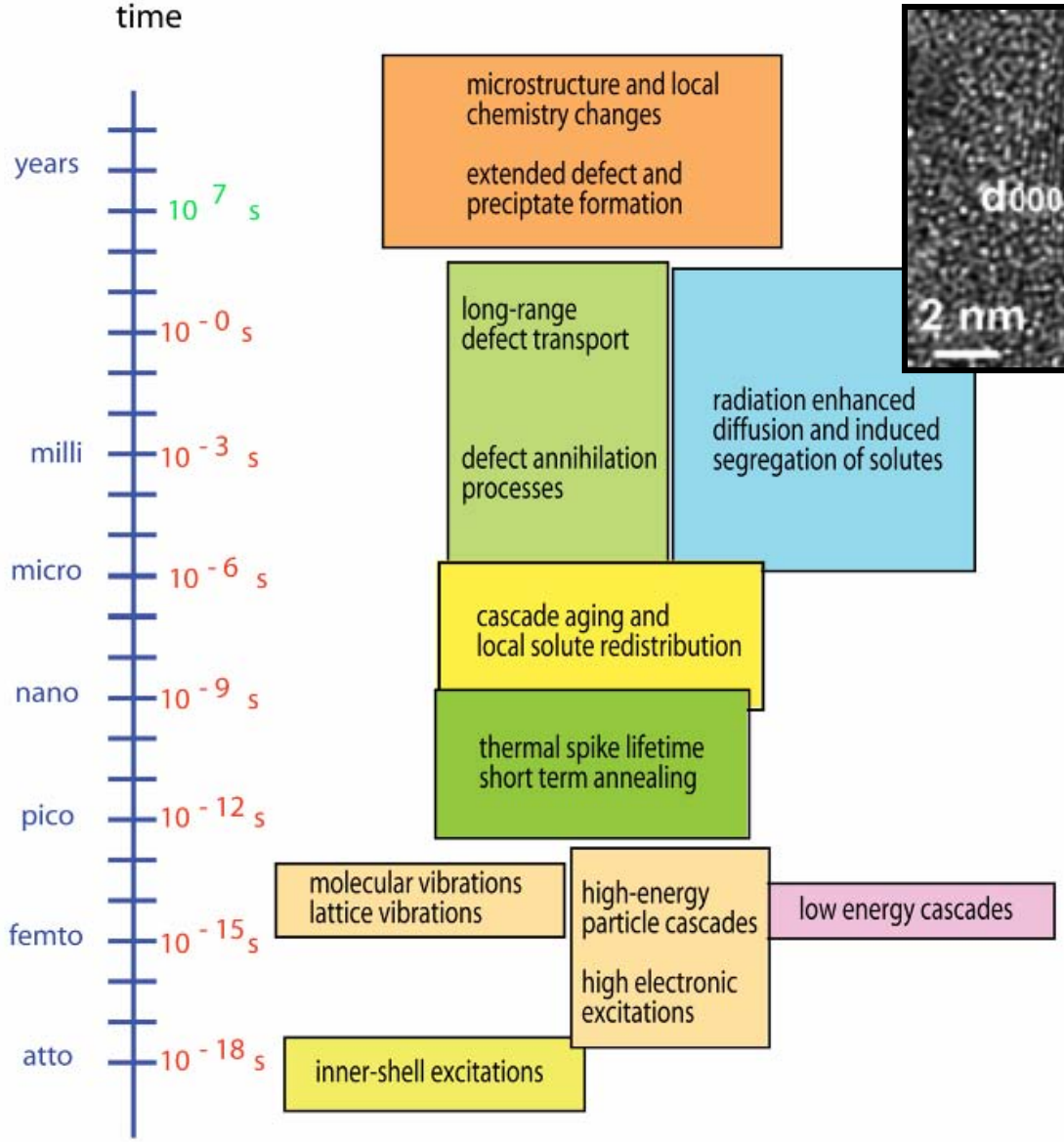


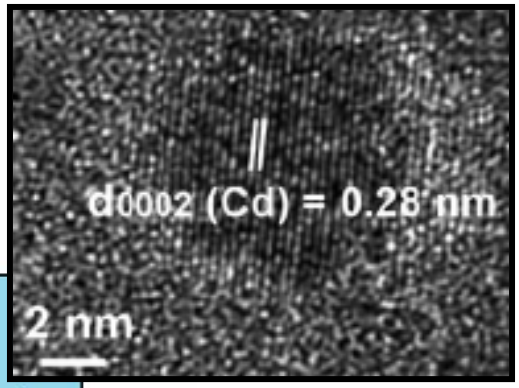
Bei, George, Pharr

Understanding of Defects, Strength, Ductility Needed at Various Length, Time Scales

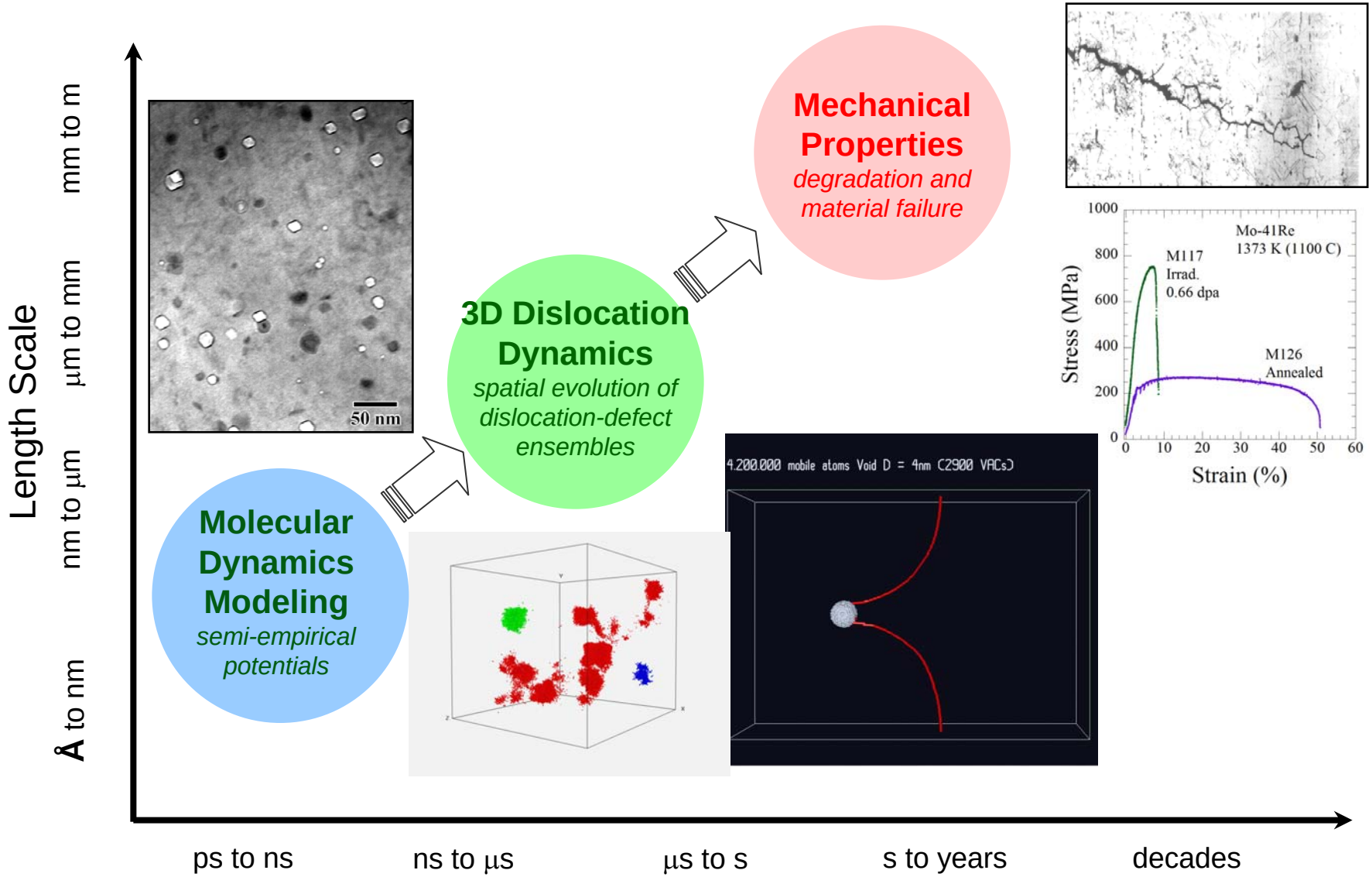


Similar Challenges Exist for Responses of Materials to Energetic Fluxes



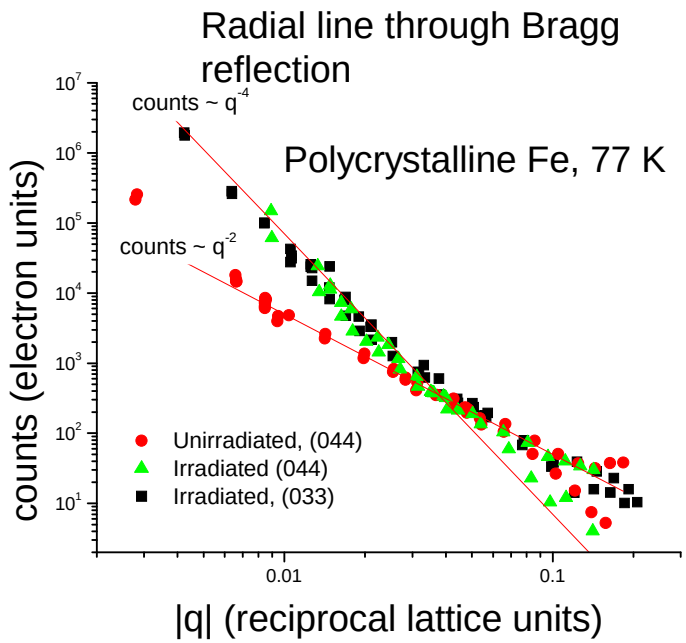


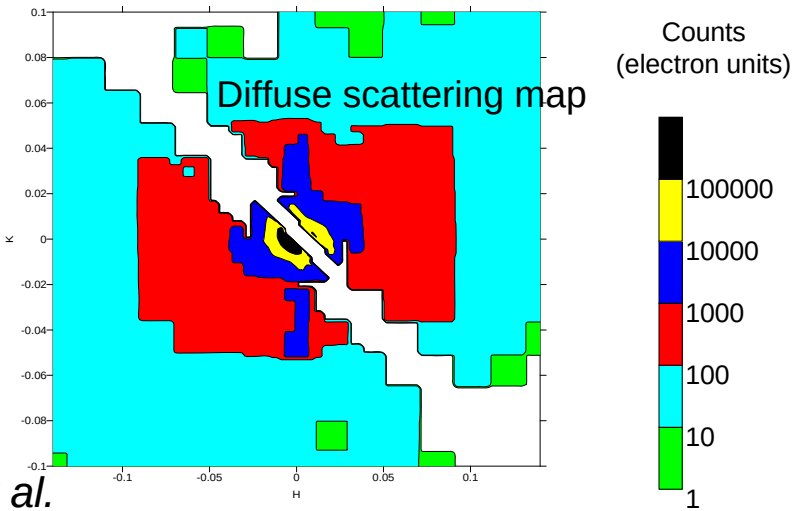
Radiation Damage: Interacting Phenomena Ranging from ps to Decades and Å to Meters



X-Ray Microdiffraction Characterizes Radiation Defects in Small Volumes

- Micron-sized irradiated samples (much lower radioactivity)
- Polycrystalline samples can be used when single crystals aren't available
- Example from a single grain in polycrystalline Fe foil
- Size, symmetry, character (vacancy/interstitial) and concentration of lattice defects measured
- Effects of 0.02 dpa proton irradiation readily measured in a 10 $(mm)^3$ volume.

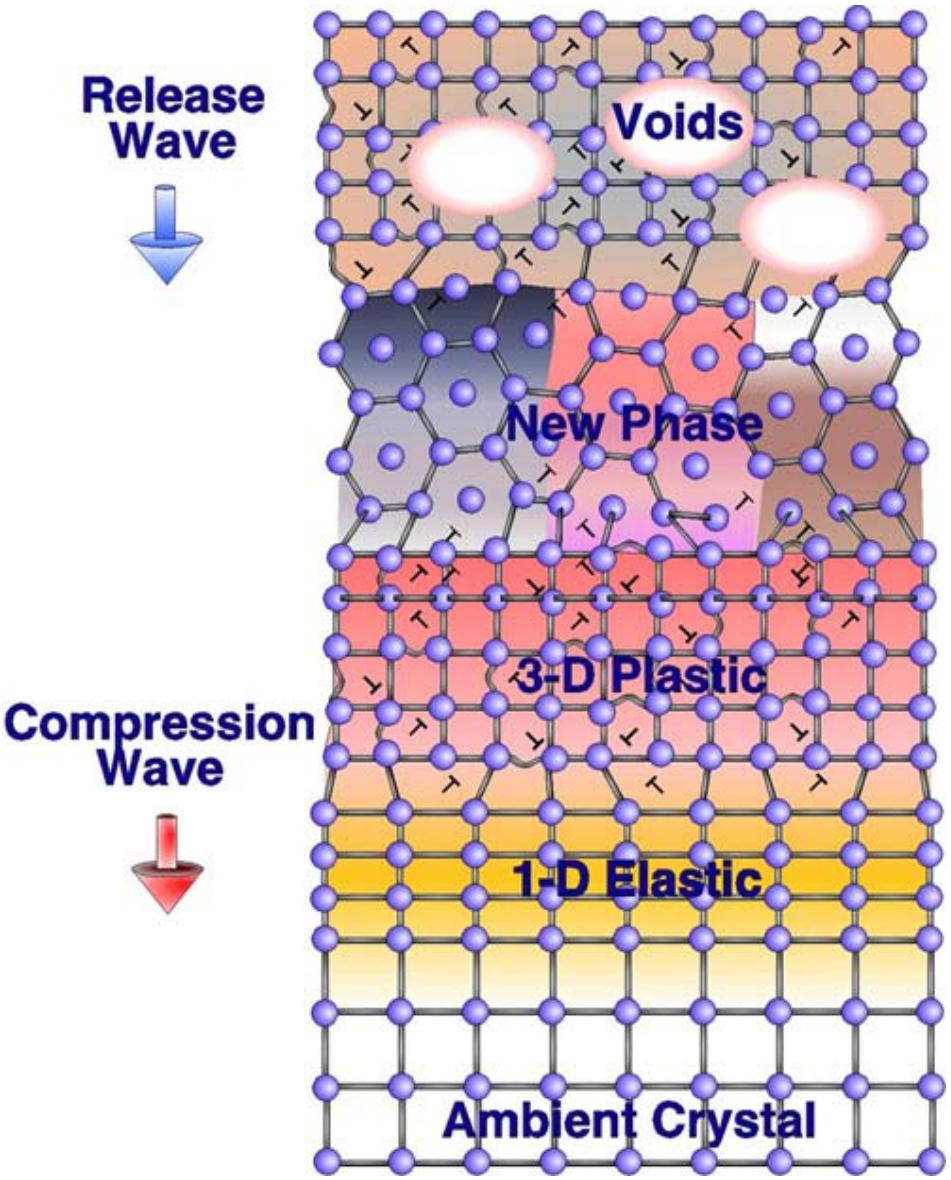




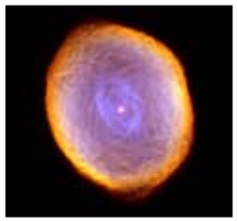
E.D. Specht et al.

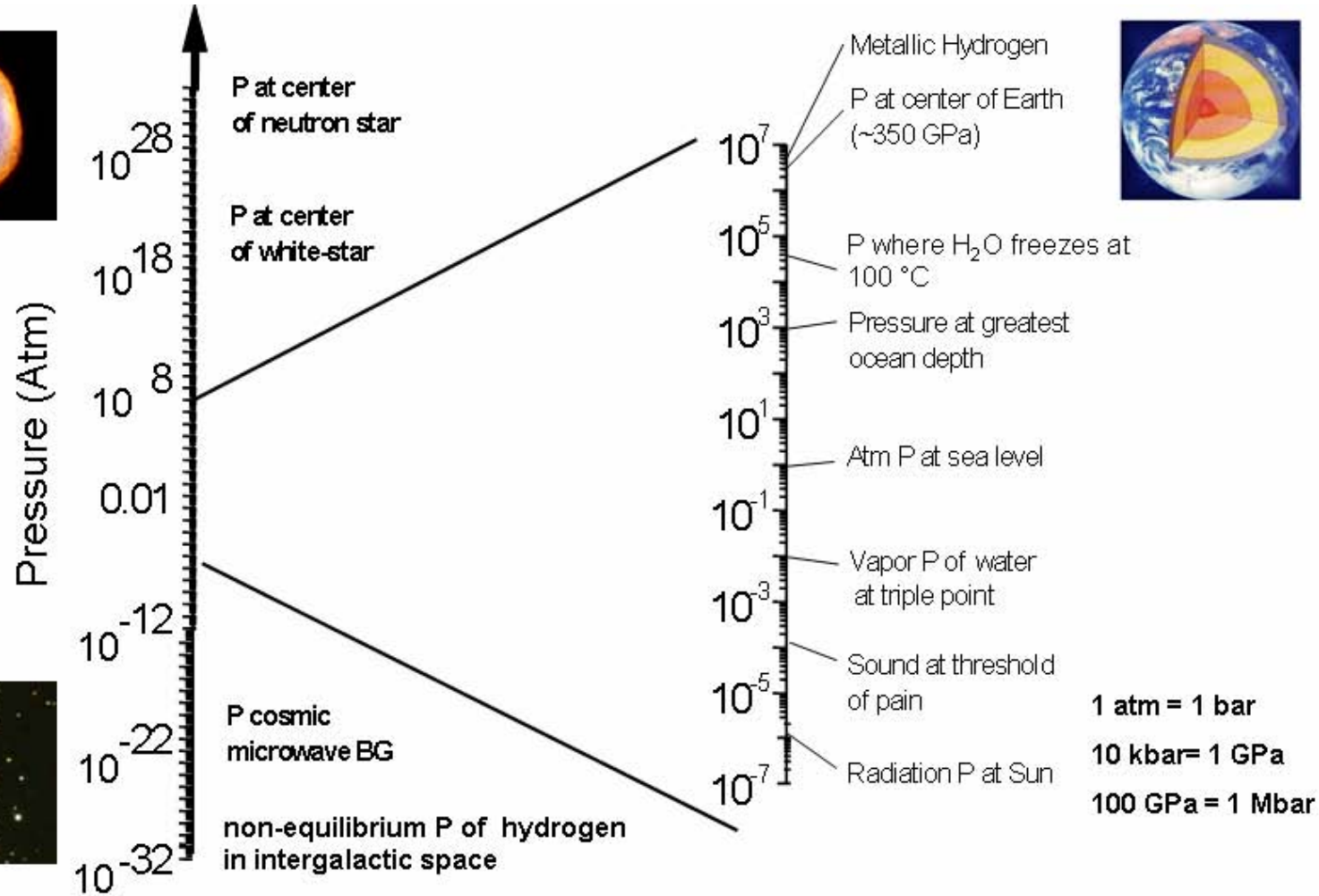
Material Response Under Highly Dynamic Stress Conditions

- Nucleation and mobility of defects and voids
- Phase nucleation and growth
- Discovery of new phenomena and material systems
- Energy absorbing structures and smart applications

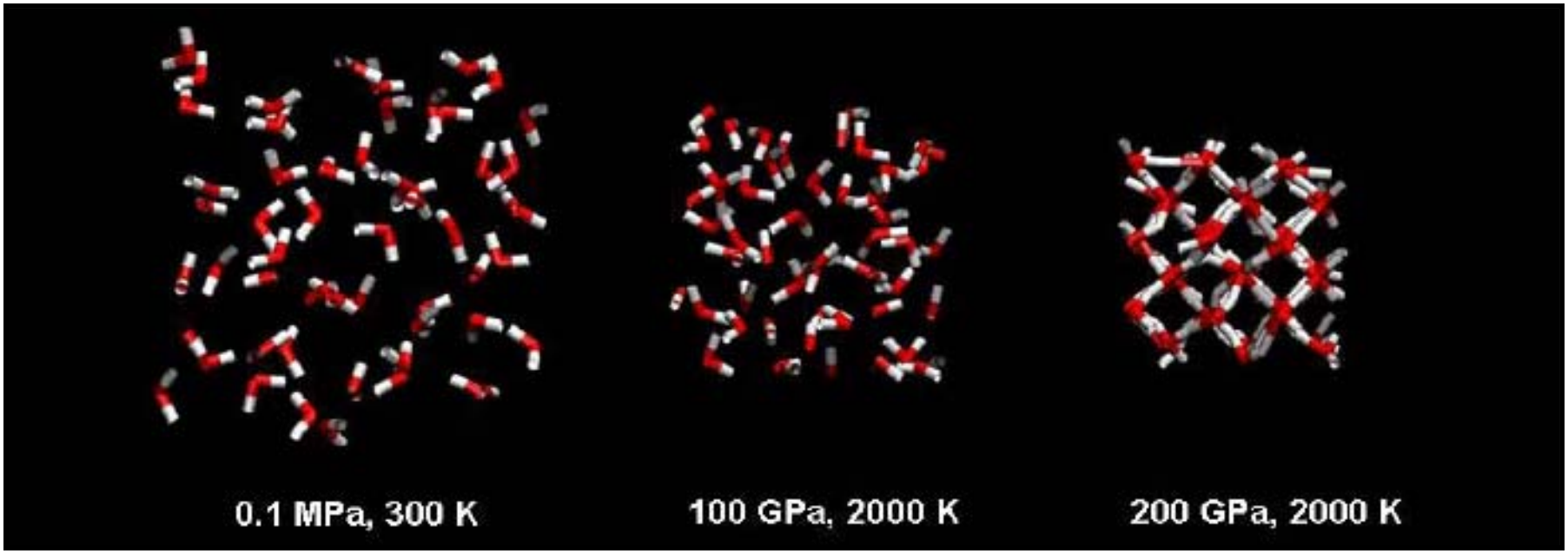


High-Pressure Research Holds Much Promise and Similar Challenges





Water Can Be Extremely Reactive at Extreme Pressures and Temperatures

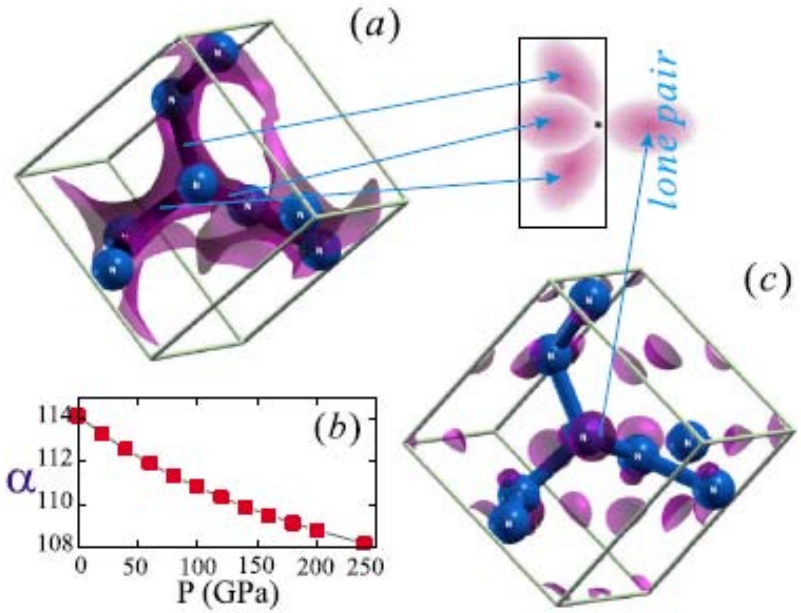


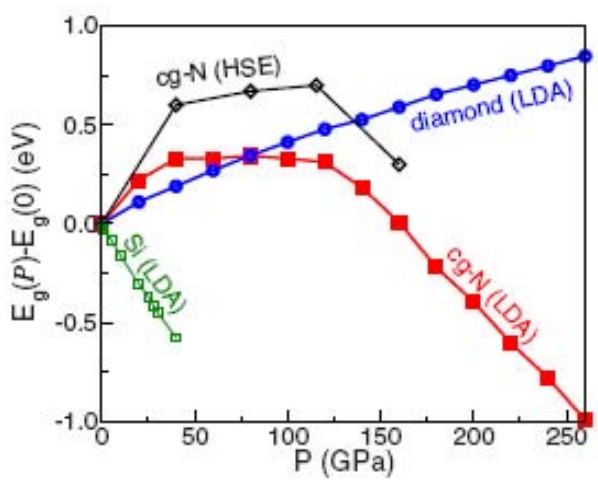
Goldman et al., 2005

Study of reaction dynamics at extremes:

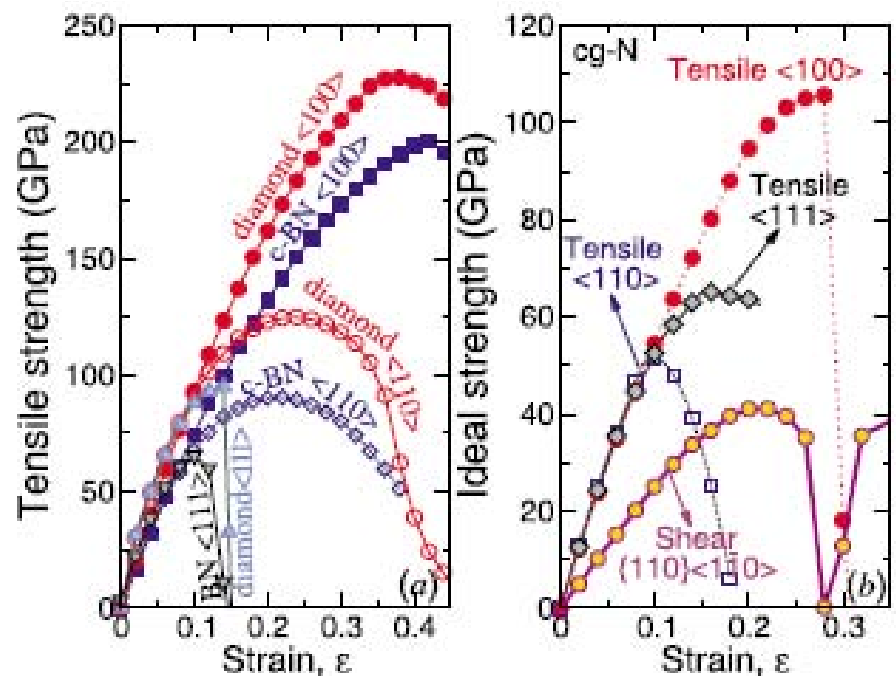
- new reaction pathways
- predictability of material reactivity at increasing levels of complexity that are strongly coupled
- understanding to control: new routes to synthesis

Bonding and Strength of Cubic Gauche Nitrogen (cg-N)





- Covalent solids with 3-fold coordination stabilized by near-tetragonal *sp*^{3}-hybridized electronic states
- Strong covalency, impressive mechanical properties

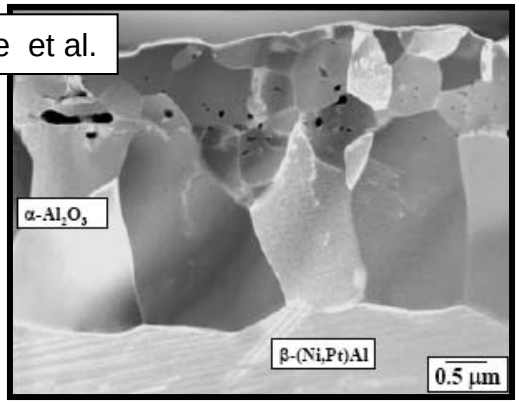


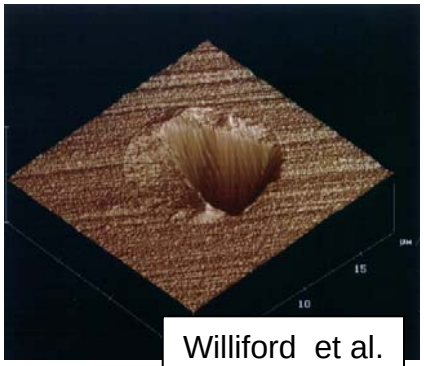
Chen, Fu, Podloucky, Phys Rev B 77 064103 (2008)

Chemically Reactive Extremes and Ideal Surface Stability

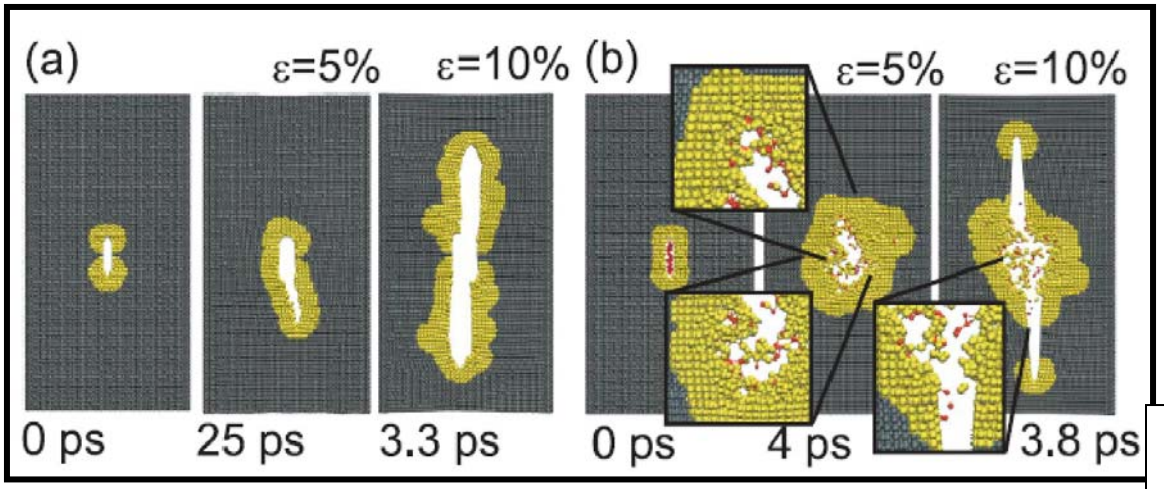
- Reaction kinetics under often severe chemical and electrochemical gradients
- Effects of reactant speciation and multiple reactants on product stability
- Reactions at fluid-solid and buried interfaces
- Properties and adherence of surface layer
- Interplay of stress-mediated changes and defects

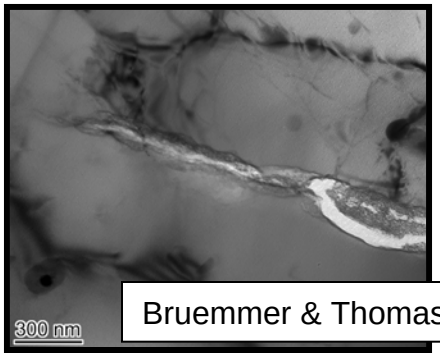
More et al.





Williford et al.



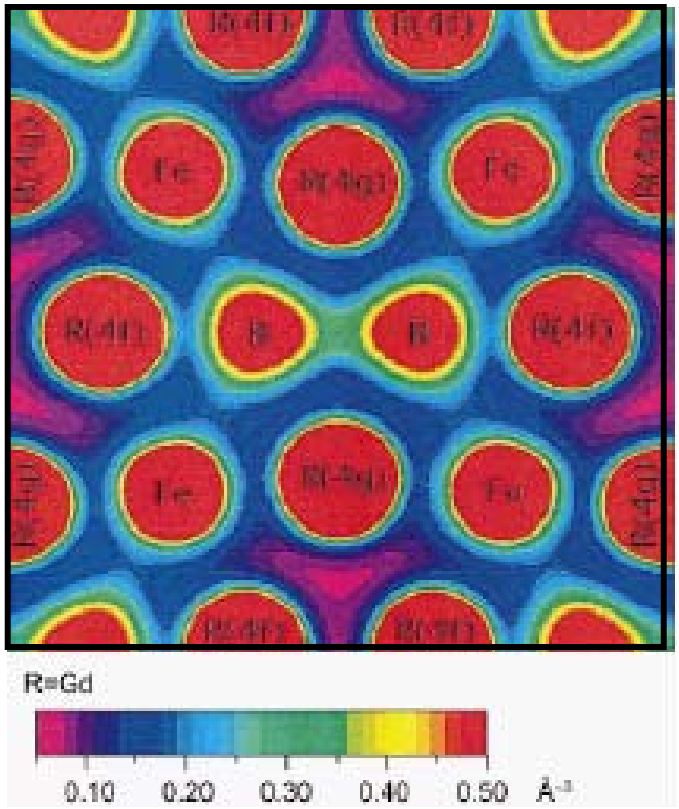


Bruemmer & Thomas

Van Duin et al.
Buehler et al..

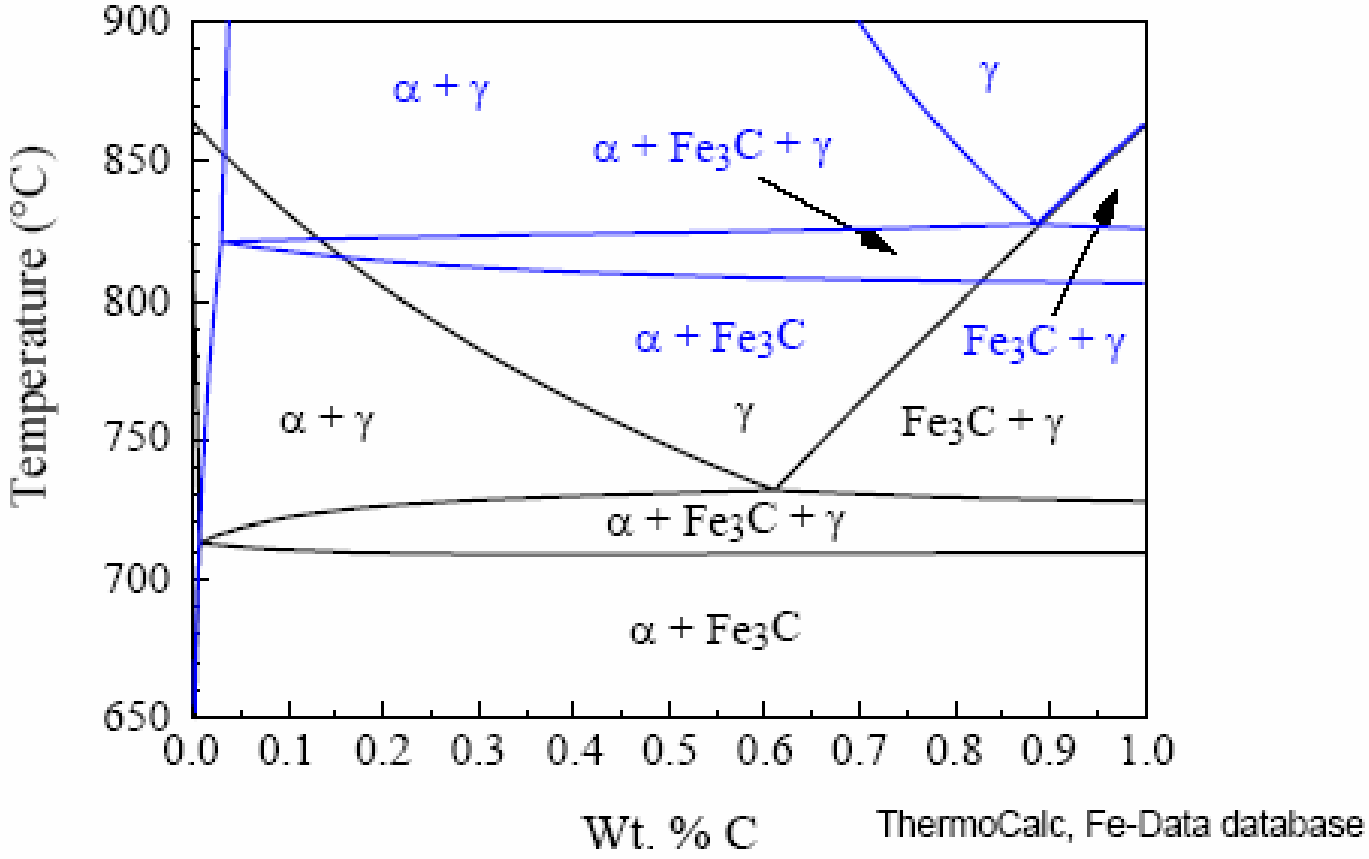
High-Performance Electrical and Magnetic Materials

- Higher electric fields: nature of breakdown
  - Atomic and nanoscale defect mechanisms
  - Local charge trapping processes
- Higher magnetic fields: permanent magnets
  - Need high density of permanent magnets
  - Fundamental electronic structure underpinnings
  - Complex crystal structures (e.g., $Nd_2Fe_{14}B$ = 68 atoms/unit cell
- Higher magnetic fields: resistive and superconducting



Yamaguchi and Asano

Much to Be Learned About Effects of Fields on Structure and Properties (Processing)



ThermoCalc, Fe-Data database

Ludtka et al.

Just Imagine the Things We Can Do!

- Think Big (Extreme)!
- Exploit new experimental, theoretical, and modeling tools matching time and length scales
- Look to
  - underpinning themes and synergies
  - performance extremes as well as effects of extreme environments
  - opportunities for materials design and synthesis