Dislocation Dynamics: Progress and Challenges

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US Fusion Materials Science Program

Strategic Planning Meeting

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Presentation Outline

- Status of Dislocation Dynamics;
- Fusion Materials Applications;
- Recent Achievements;
- Challenges, Limitations & Future Directions:
  - Near-Term (1-3 years);
  - Long-Term (> 3 years).

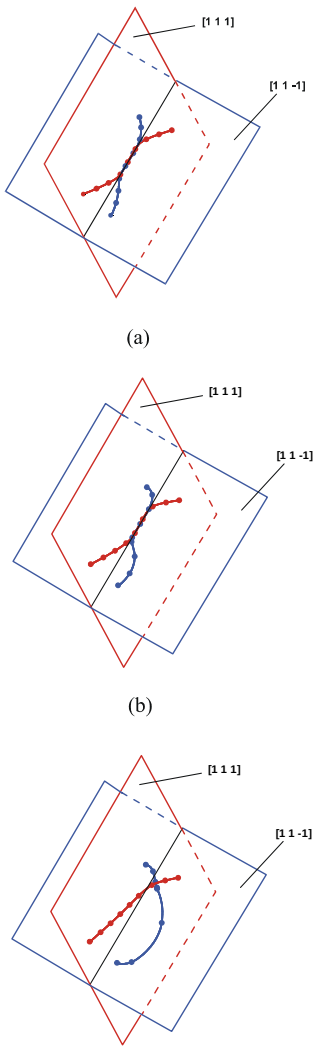
Status of Dislocation Dynamics

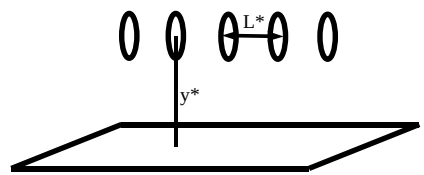
- **The Objective of DD is the development of Physically-Based Computer Simulations of Plasticity and Fracture Processes in Fusion Materials;**
- **Eliminate Atomic Degrees of Freedom;**
- **Develop "Ab initio elasticity-based" simulations (i.e. no rules);**
- **Input Parameters are few:**
  - **Elastic Constants (well-known);**
  - **Dislocation Mobility (experiment/ MD / ab-initio simulations).**
- **The Method has World-Wide Appeal:**
  - Lattice Methods (Kubin, Canova, Devincre, …..)
  - Force Methods (Zbib, Hirth, Bulatov, Rhee, ….)
  - Differential Stress Methods (Schwarz, Tersoff, LLNL folks, ….)
  - Parametric Dislocation Dynamics, PDD (Ghoniem, Sun, Huang, …)
  - Phase Field Methods (Khatchaturian, Wong, …).

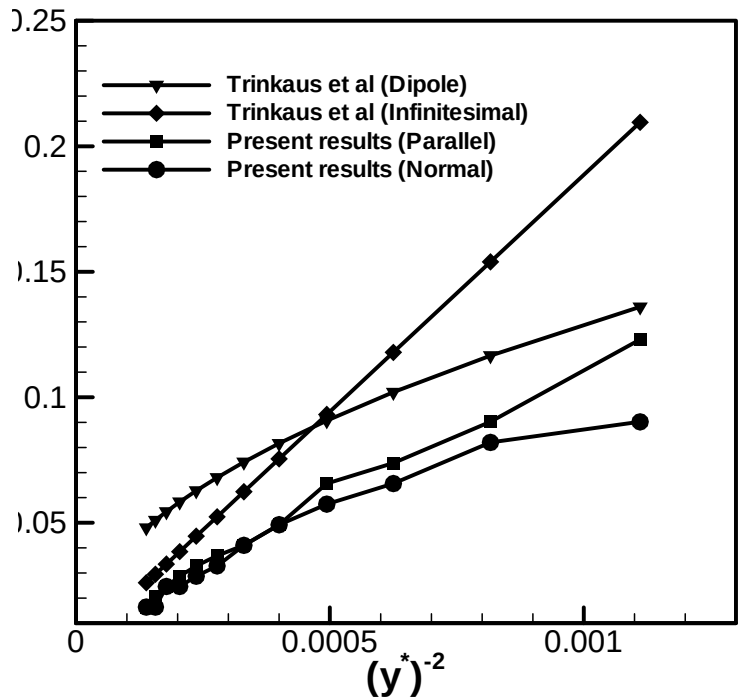
Fusion Materials Applications

1) Dislocation-Microstructure Interaction (SIAs, SFTs, Voids, Bubbles, Precipitates, and Grain Boundaries);
2) Deformation Mechanisms (e.g. Flow Localization, Fracture);
3) Constitutive Modeling (e.g. stress-strain-temperature-strain rate-flux-fluence relationships);
4) Understanding of Experimental Observations (e.g. Radiation Hardening & Softening);
5) Experimental Design of Innovative Materials (e.g. Thin Films & Nano-layers);
6) Material Design (Alloying, microstructure distribution, grain size, nano-laminates, etc.)

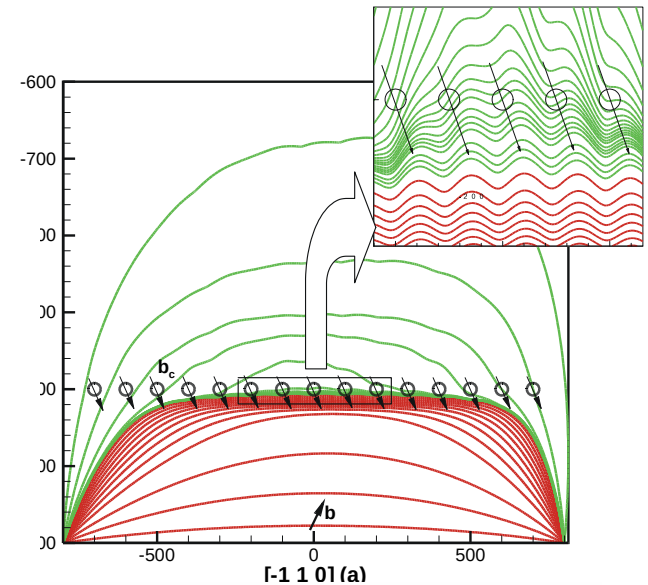
Application (1): Dislocation-Microstructure Interaction

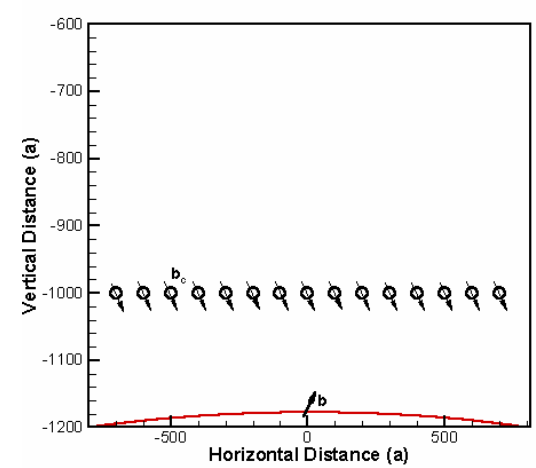




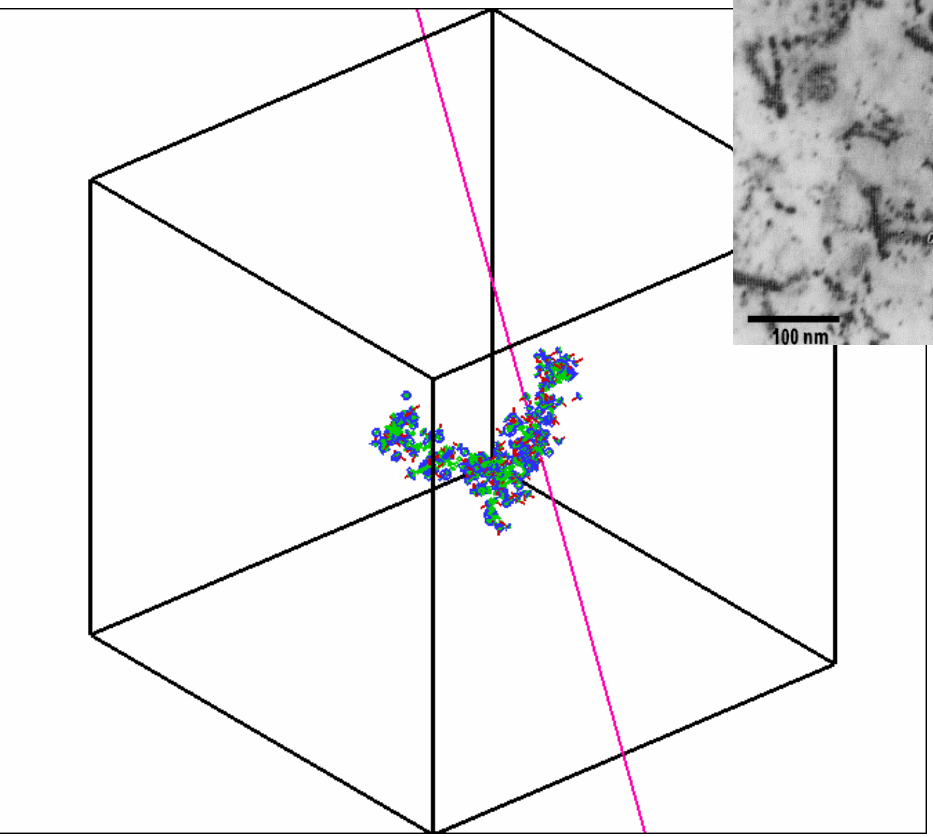


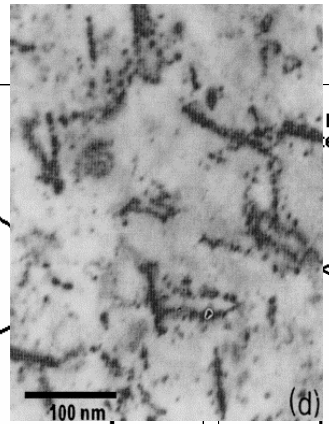
Flow Stress Scaling

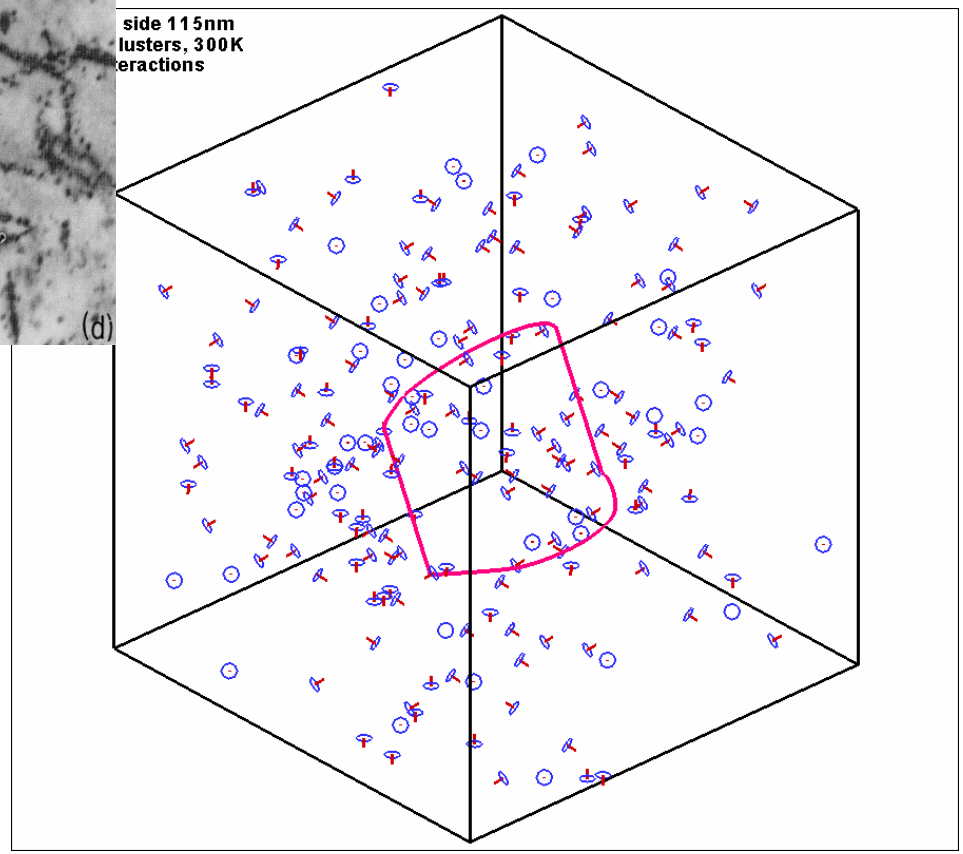




Dislocation-Microstructure Interaction: KMC Modeling of Pinning and Rafting





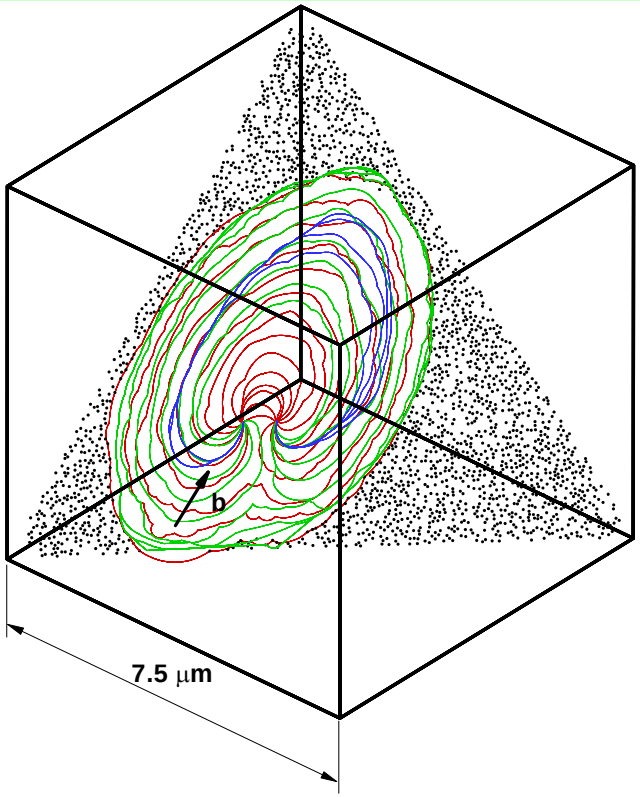


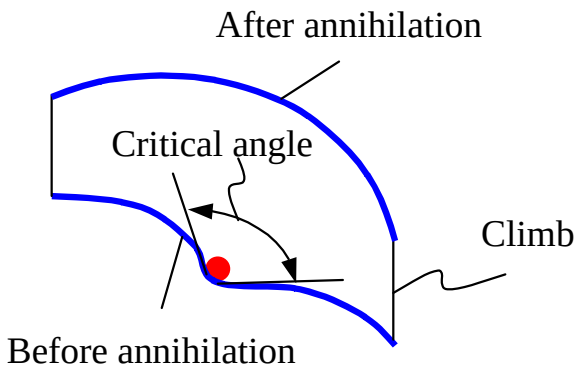
In collaboration with RISO (Singh) & ORNL (Stoller/ Osetsky)

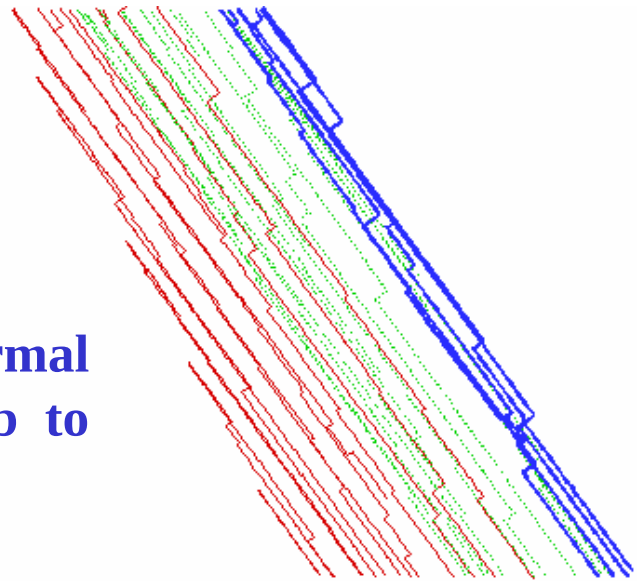
Limitations and Future of Dislocation-Microstructure Interaction

- **Status:**
  - Rigorous dislocation-dislocation, and dislocation-SIA (isotropic);
  - Approximate for SFT, voids, and precipitates;
  - Stochastic (KMC) and thermally-activated started;
  - Time scale problem for microstructure evolution is not solved;
  - Limited study of interaction with "defect atmospheres"
- **Future Plans:**
  - Anisotropic elasticity;
  - Rigorous simulations for SFTs, voids and precipitates;
  - Dislocation-grain boundary interactions.
  - Microstructure cutting and sweeping (e.g. voids, bubbles and precipitates).

Application (2): Flow Localization & Fracture







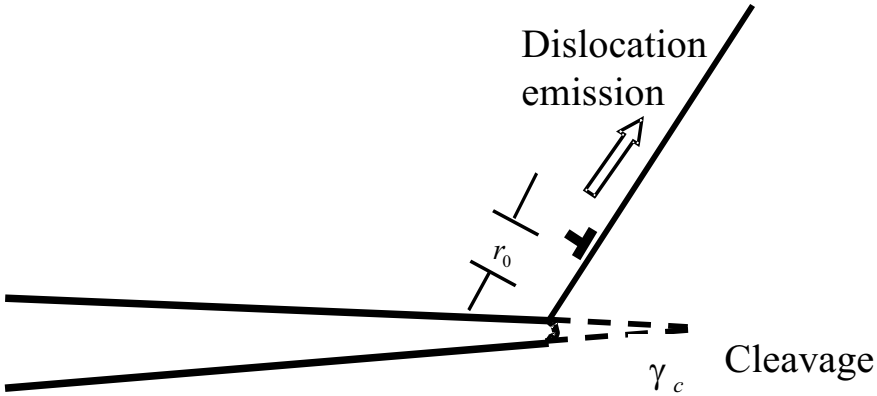
<u>Mechanism:</u> (1) glide, (2) local thermal destruction of vacancy clusters, (3) climb to widen channel.

In collaboration with RISO (Singh) & PNNL/ORNL (Edwards/ Zinkle)

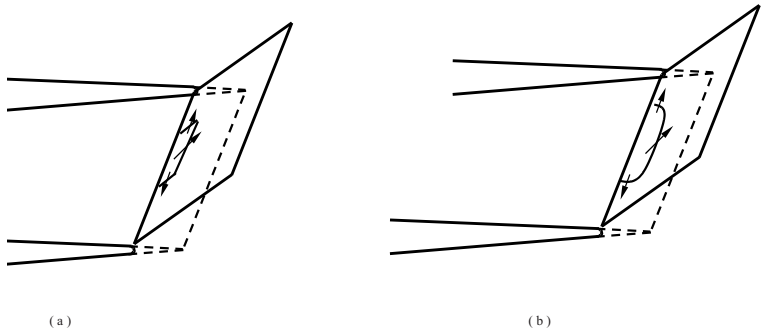
Limitations and Future of Flow Localization

- **Status:**
  - Two explanations for channel width: (1) climb/glide/localized thermal dissolution (Ghoniem et al.), (2) dipole width (Zbib et al);
  - Both are not totally consistent with available data;
  - MD results do not show SFT destruction;
  - No conclusive explanation for inter-channel length scale;
  - Channel source, termination and dynamics (i.e. time scale) not clear.
- **Future Plans:**
  - Extend the "hot spot" avalanche pileup theory of Armstrong, Head, et al. (Eglin Air force Base);
  - Simulation of avalanche time evolution and comparison with Neuhauser;
  - Coupled DD/ mesh-free simulations for inter-channel length scale.

Research on Fracture Modeling



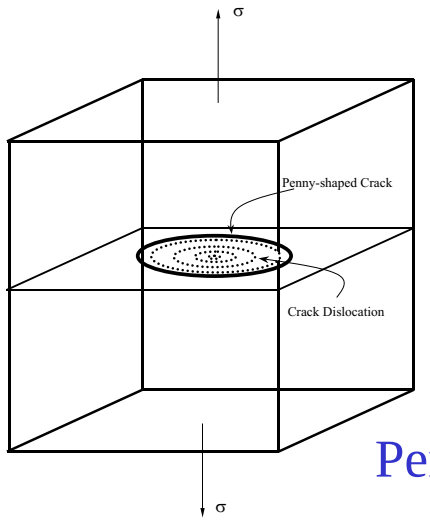
Rice-Thomson Model



Pseudo-3D Emission Model

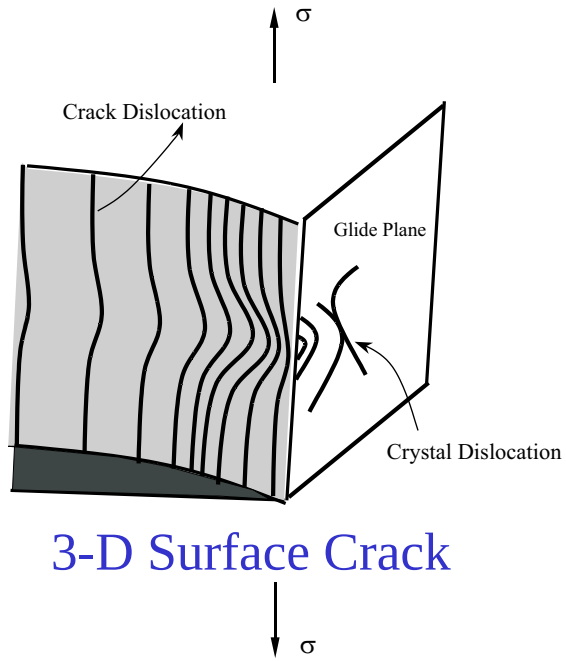
Small Value in $\mu b/\gamma_c$ & Wide

Dislocation Core → Ductile



Penny-Shaped Crack

Collaboration:
Odette et al (UCSB)

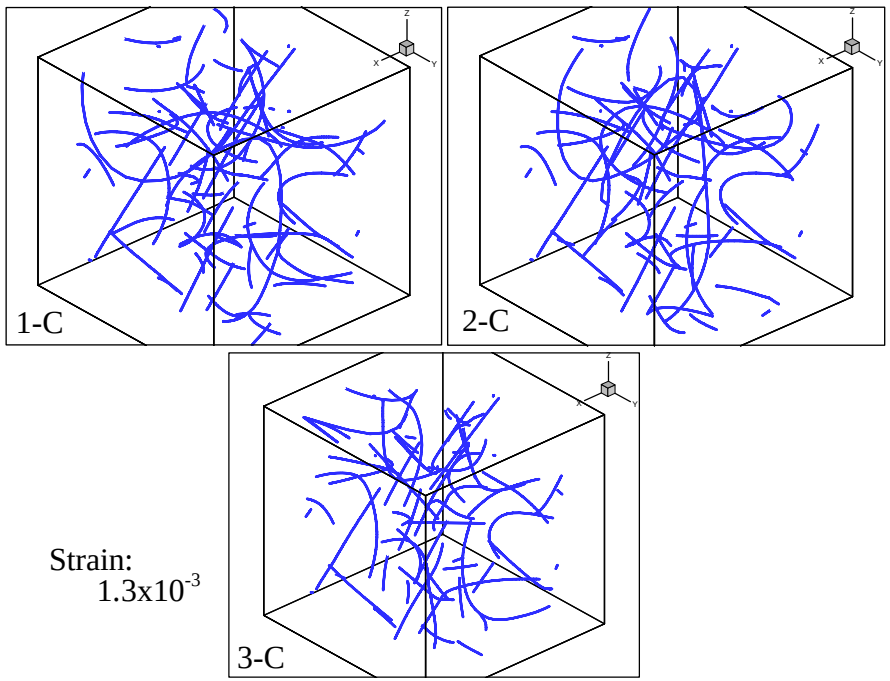


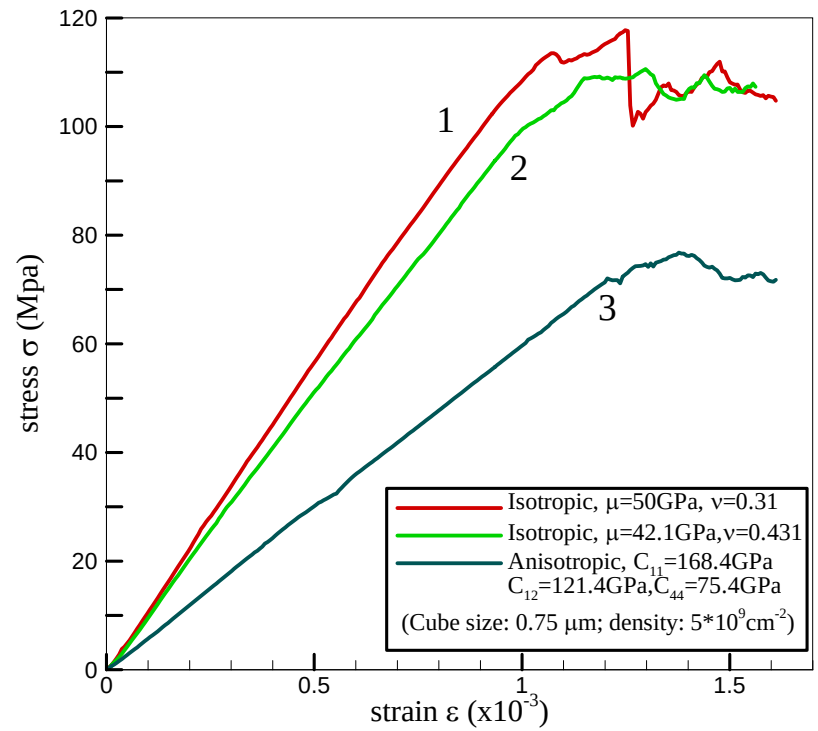
3-D Surface Crack

Status & Future Plans of Fracture Modeling

- **Status:**
  - J. Huang (PhD) started modeling true 3-D cracks as "Parametric Dislocation Pileups,"
  - S. Nooronha (post-doc, Hirsch) started to couple ABACUS elasto-plastic FEM with the Oxford 2-D dislocation emission at precipitates;
  - Effective dislocation mobility in a random field of SFTs/ voids.
- **Future Plans:**
  - Model Fracture specimens at UCSB for pure Fe & ferritic steels;
  - Determine DBTT shifts and consistency with Master Curve method;
  - Investigate 3-D aspects (e.g. crack shape, stress triaxiality, surface/ embedded flaws, etc.)

Application (3): Constitutive Modeling & Anisotropic DD





Anisotropic Single Crystal Deformation and Microstructure are significantly different from the isotropic case.

Limitations and Future of Constitutive Modeling

- **Status:**
  - Single Crystal (Isotropic & anisotropic)
  - Small strain (<1%);
  - Small volume (<1 micron);
  - Single Processor (~1 day/ case).
- **Near-Term Progress (1-3 yrs):**
  - Parallel Code Completed;
  - LeSar/ Rickman Far-Field Method Implemented;
  - Computer Science Approaches Started (Load Balancing, Near-neighbor Searches, Cluster Computing efficiency);
  - Will be deployed on the ISIS Beowulf Cluster at UCLA.

Long-Term Goals of Constitutive Modeling

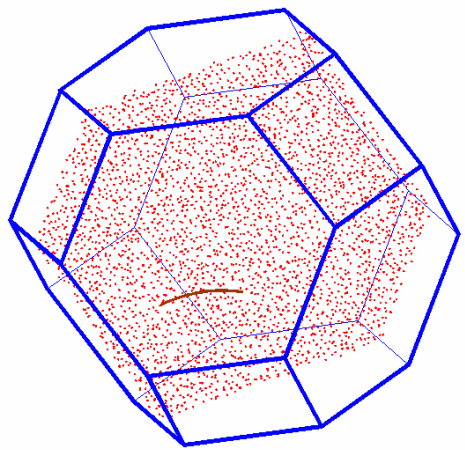
1) Efficient, Experimentally Calibrated Parallel Code for Single Crystals;

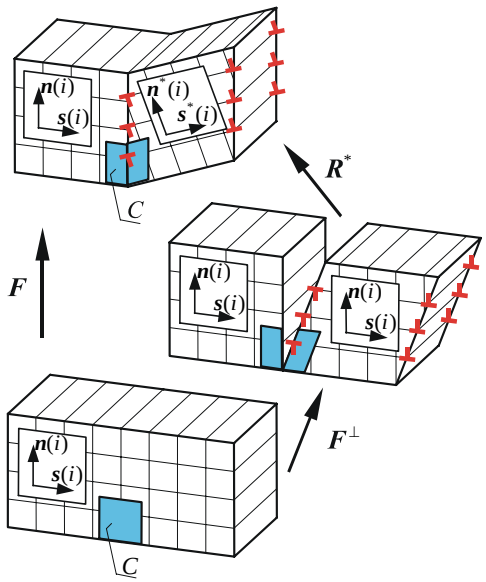
2) Coupling between Crystal Plasticity and DD;

3) Development of Polycrystal Plasticity Code with Grain Boundary Evolution;

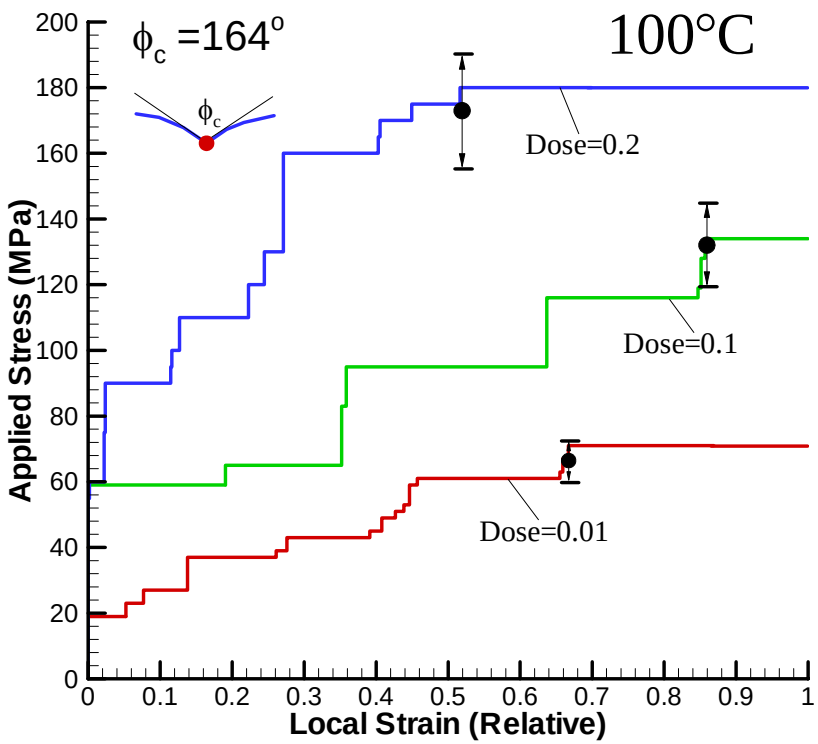
4) Coupling with: (a) Mesh-Free for Flow Localization, (b) FEM for Design;

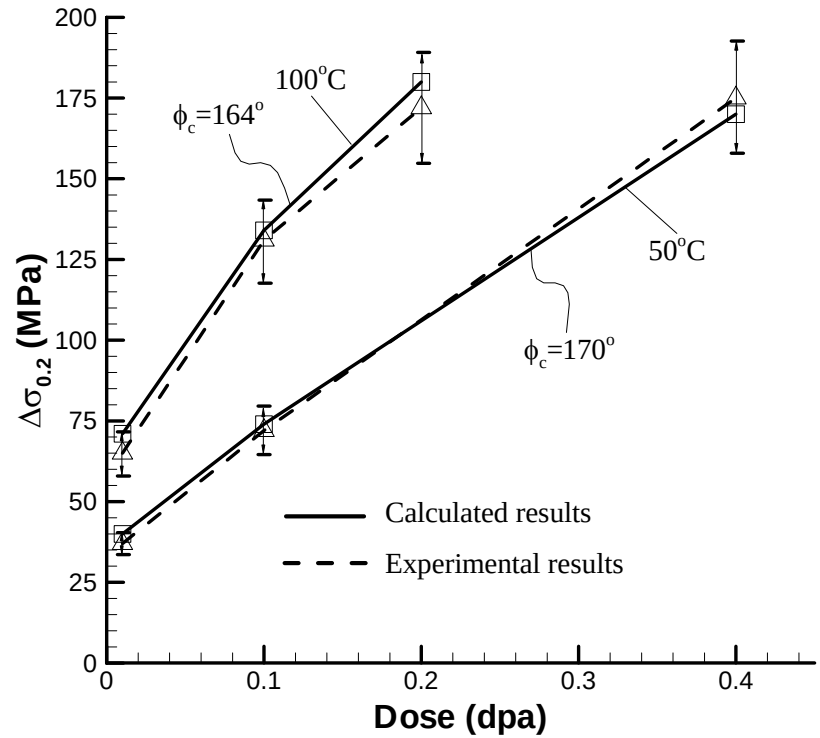
5) Continuum alternative requires vast data base and "ad hoc" assumptions.





Application (4): Understanding Experiments on Radiation Hardening & Softening

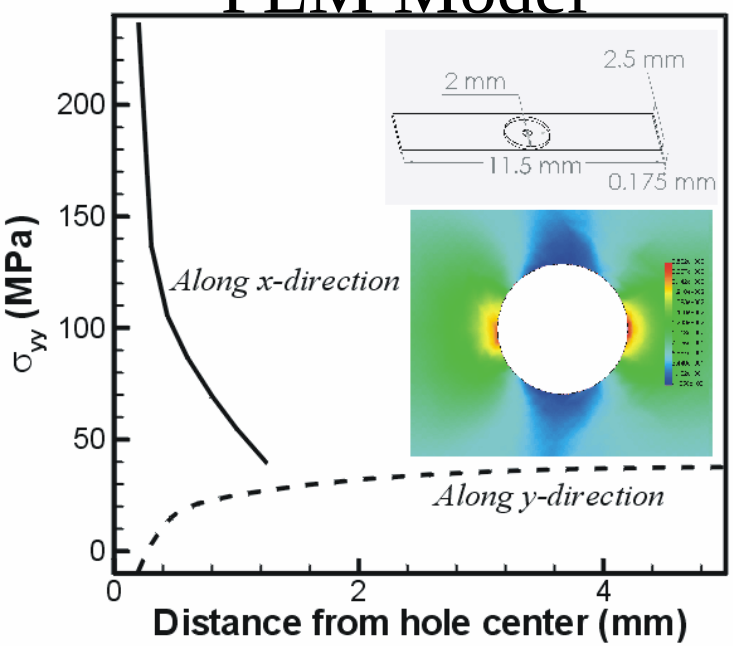


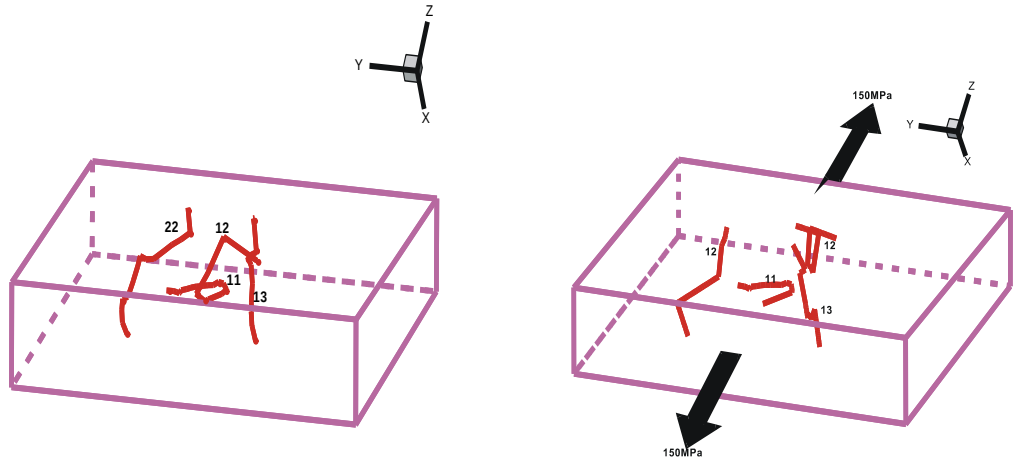


In collaboration with RISO (Singh) & PNNL (Edwards)

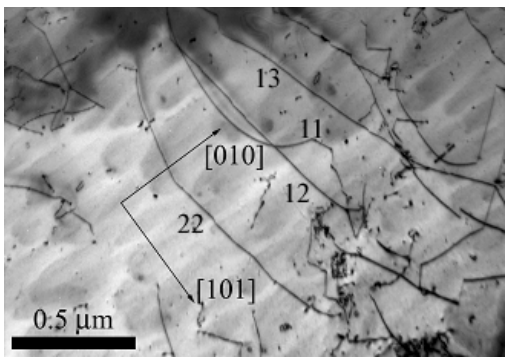
Application (5): Experimental Design of Innovative Materials (Stereographic TEM of Thin Films)

FEM Model



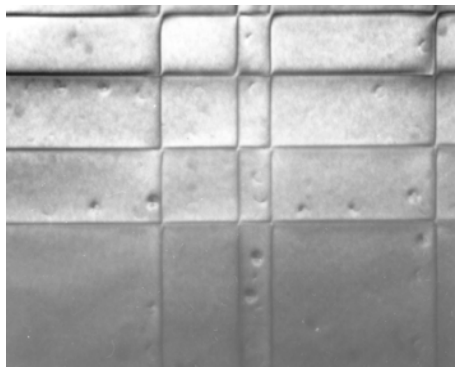


Initial and deformed configurations

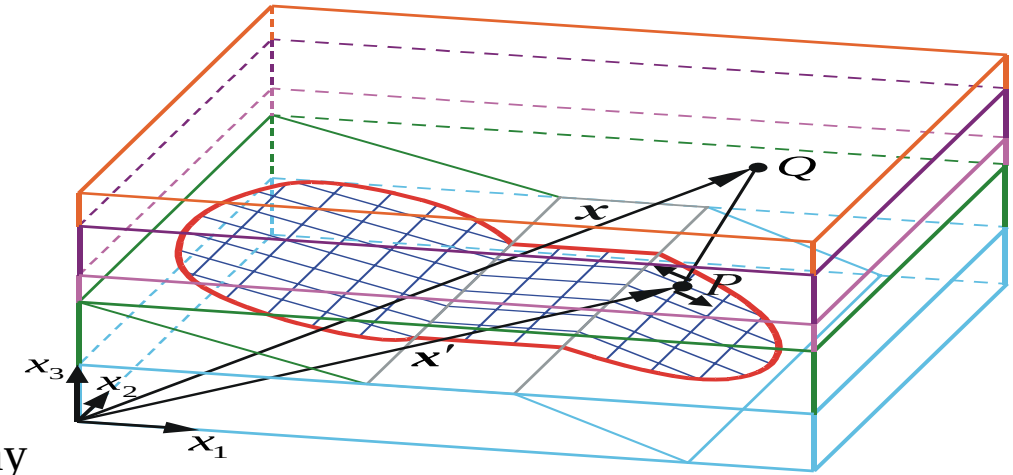


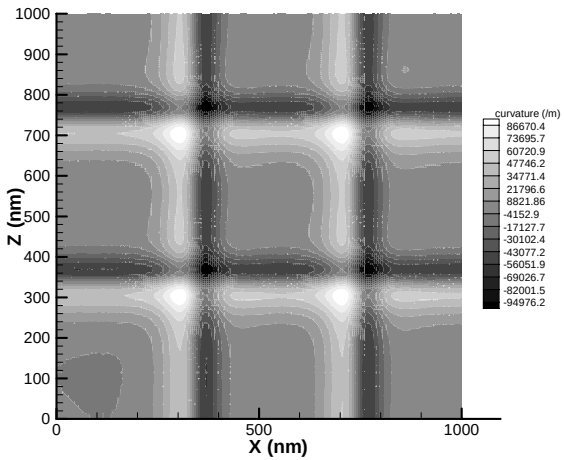
In collaboration with LANL (McCabe, LeSar, Misra & Mitchell

Application (6): Ultra-strong Material Design

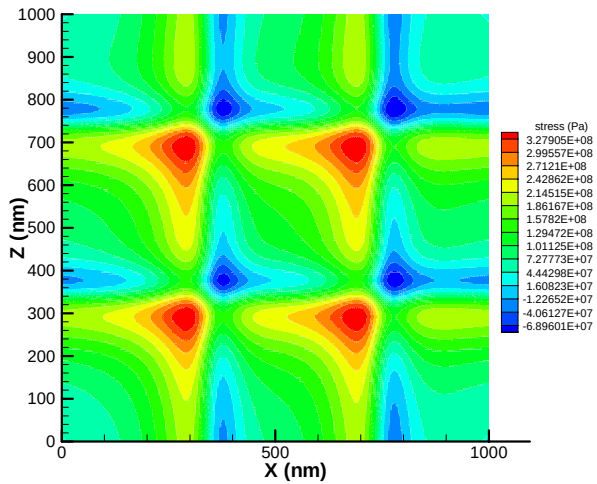


Experimental TEM interfacial array





Calculated interfacial array curvature map



Interfacial in-plane Stress Map