MESOSCOPIC MODELS OF DEFORMATION AND FRACTURE OF FUSION MATERIALS

Presented by

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Contributors

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Fusion Materials Program Review at UCSB

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Presentation Outline

- Mechanisms of plastic instabilities
- Plastic flow localization in irradiated materials
- Mesoscopic computer simulations & DD
- Dislocation interaction with defect clusters
- Radiation hardening & embrittlement by flow localization
- Application to flow localization of irradiated copper and iron
- Fracture Toughness models
- Conclusions and future directions

SUMMARY

Title of Work: **Plasticity and Fracture Mechanisms of Fusion Materials**

Principal Investigator and Institution: **Nasr M. Ghoniem (UCLA), Hussein Zbib (WSU), Brian Wirth (LLNL), G.R. Odette (UCSB), D. Edwards (PNNL), S. Zinkle (ORNL)**

Overall Objective: **Computer Modeling and mechanistic experiments of the main phenomena involved in plastic flow localization and associated fracture instabilities under irradiation.**

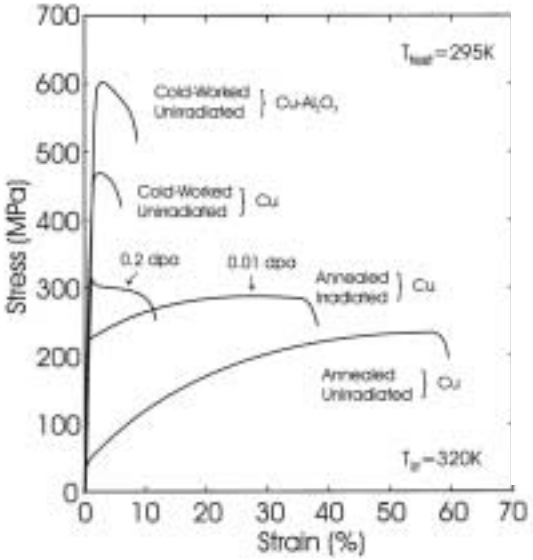
Technical Approach: (1) Dislocation Dynamics Modeling; (2) Experimental Data Assessment; (3) Mechanisms of failure models; (4) mechanistic experiments.

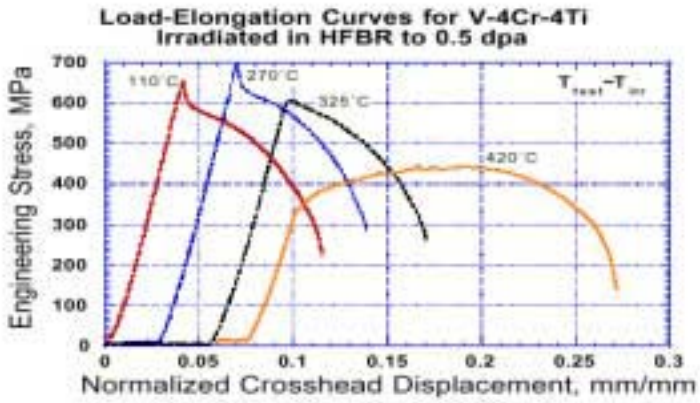
Accomplishments:

- Established the main mechanisms of dislocation-defect interactions;
- Developed new computational tools for simulations of plastic flow;
- Established the main mechanism of plastic flow localization.
- Coordinated effort with the experimental program.

Relevance to OFES/Fusion: **Mechanistic understanding of flow and fracture is essential to successful alloy development.**

Technological Motivation Behind Mesoscale Simulations



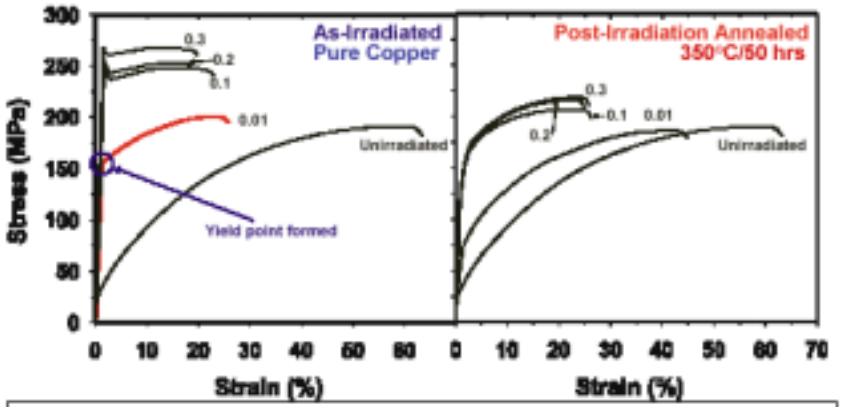


Plastic Instability

Flow Localization

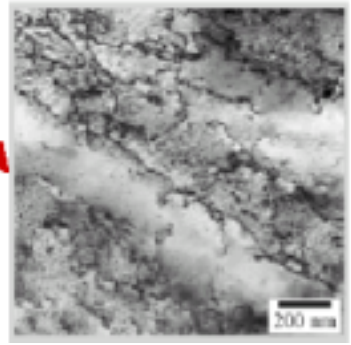
(1) Exposure of pressure vessel steels in nuclear fission reactors leads to severe embrittlement affecting safety and economics.
(2) Irradiated metals in future fusion energy sources undergo plastic flow localization instabilities.

Deformation Behavior in As-irradiated and Post-irradiation Annealed Pure Cu



As-Irradiated, 0.3 dpa

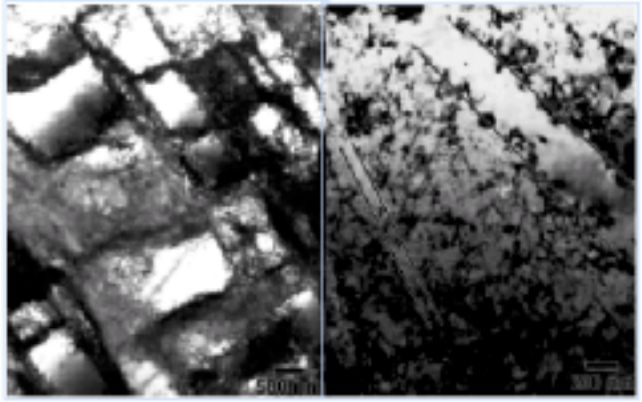
- Cleared channels with little to no dislocation movement between the channels; localized deformation
- Large increases in strength (6 to 8x)
- Loss of uniform elongation and work hardening capacity
- Formation of a clearly defined yield point



Post-Irradiation Annealed Condition

- Dislocation cell structure: material deforms homogeneously at 0.01 dpa
- Mixture of channeling and homogeneous deformation at 0.3 dpa

PI Annealed, 0.01 dpa | PI Annealed, 0.3 dpa



Battelle

U.S. Department of Energy
Pacific Northwest National Laboratory

Mechanisms of Plastic Instabilities

$$d\sigma = h\, d\varepsilon + S\, d(\log \dot{\varepsilon})$$

Strain hardening rate

Strain rate sensitivity

$$\lambda = [(\sigma - h) / S]\, \dot{\varepsilon}$$

Stable Plastic Flow → $\lambda < 0$

Unstable Plastic Flow → $\lambda > 0$

Basic Equations of Differential Geometric Curved Segments

Differential Geometry

$$(\mathbf{a}_1 = \mathbf{e},\ \mathbf{a}_2 = \mathbf{t},\ \mathbf{a}_3 = \mathbf{b}) \qquad \mathbf{e} = \frac{\mathbf{R}}{R} \qquad \mathbf{t} = \frac{\mathbf{T}}{T} \qquad \mathbf{T} = \frac{d\mathbf{l}}{dw}$$

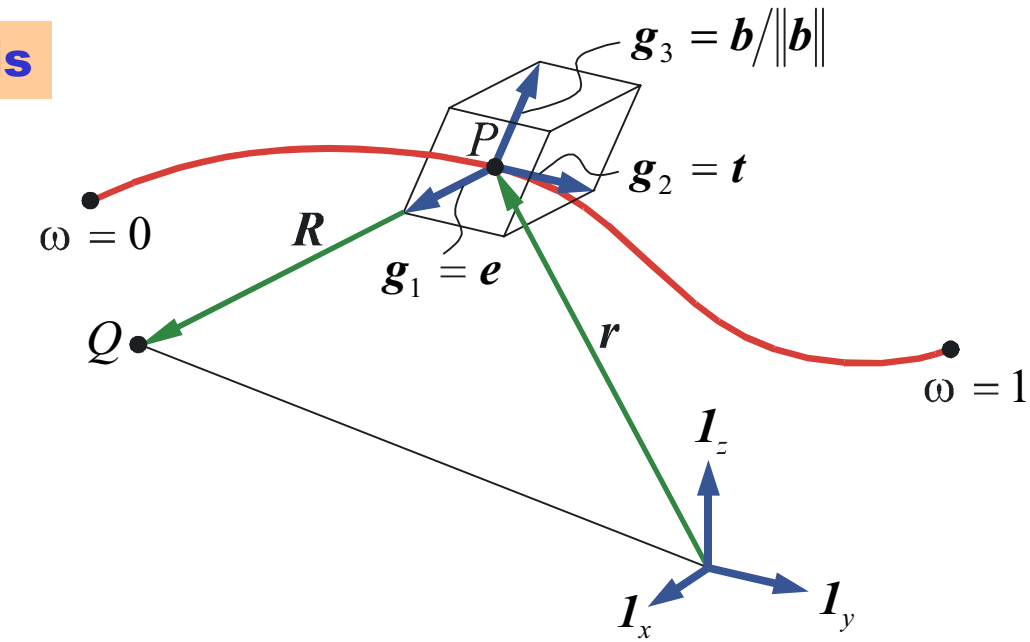
Contravariant Vector Basis

$$\mathbf{a}^1 = \frac{1}{2\pi V}(\mathbf{a}_2 \times \mathbf{a}_3)$$

$$\mathbf{a}^2 = \frac{1}{2\pi V}(\mathbf{a}_3 \times \mathbf{a}_1)$$

$$\mathbf{a}^3 = \frac{1}{2\pi V}(\mathbf{a}_1 \times \mathbf{a}_2)$$

$$V = (\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3$$



Basic Equations of Differential Geometric Curved Segments

Equations of Motion

$$\int_{\Gamma} \left(f_k^t - BV_k \right) \delta r_k \left| ds \right| = 0$$

Define:

$$r^* = \frac{r}{a} \qquad f^* = \frac{f}{\mu a} \qquad t^* = \frac{\mu t}{B}$$

Final Equation of Motion

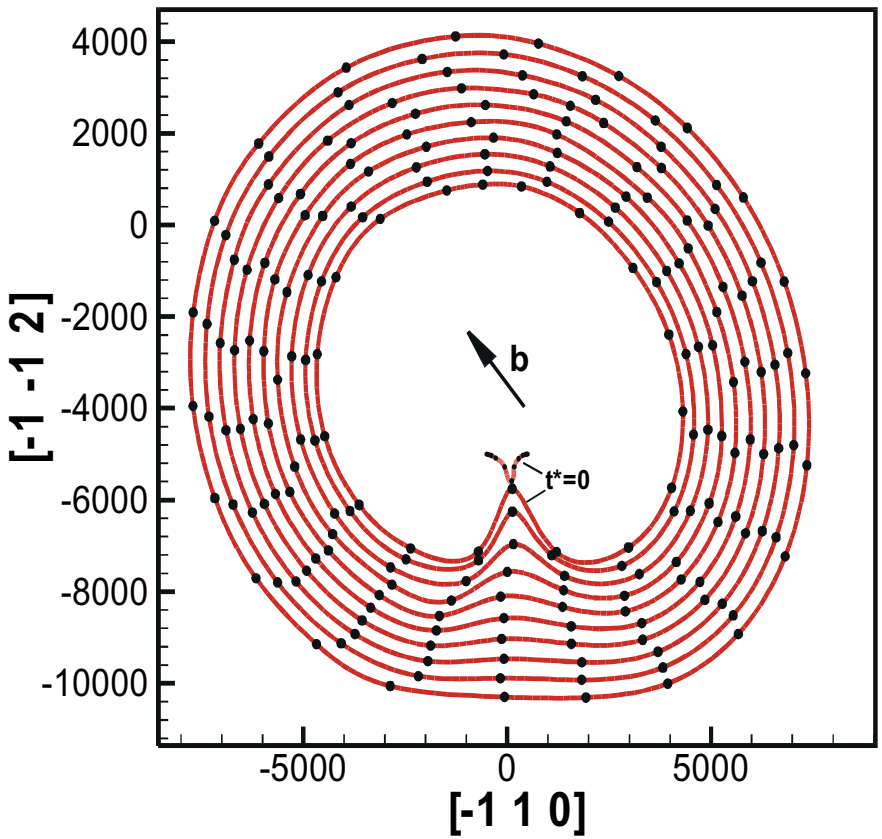
$$\mathbf{K} \frac{d\mathbf{Q}}{dt^*} = \mathbf{F} \qquad \mathbf{Q} = \left[\mathbf{P}_1, \mathbf{T}_1, \mathbf{P}_2, \mathbf{T}_2 \right]$$

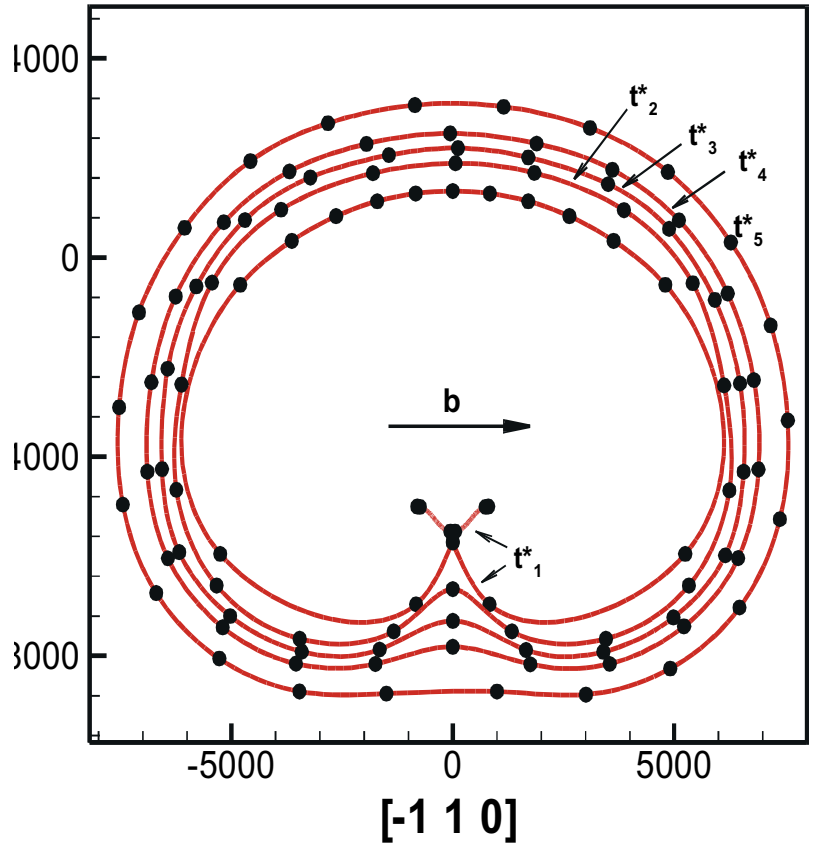
Q=Nodal coordinate vector

F=Nodal Forces

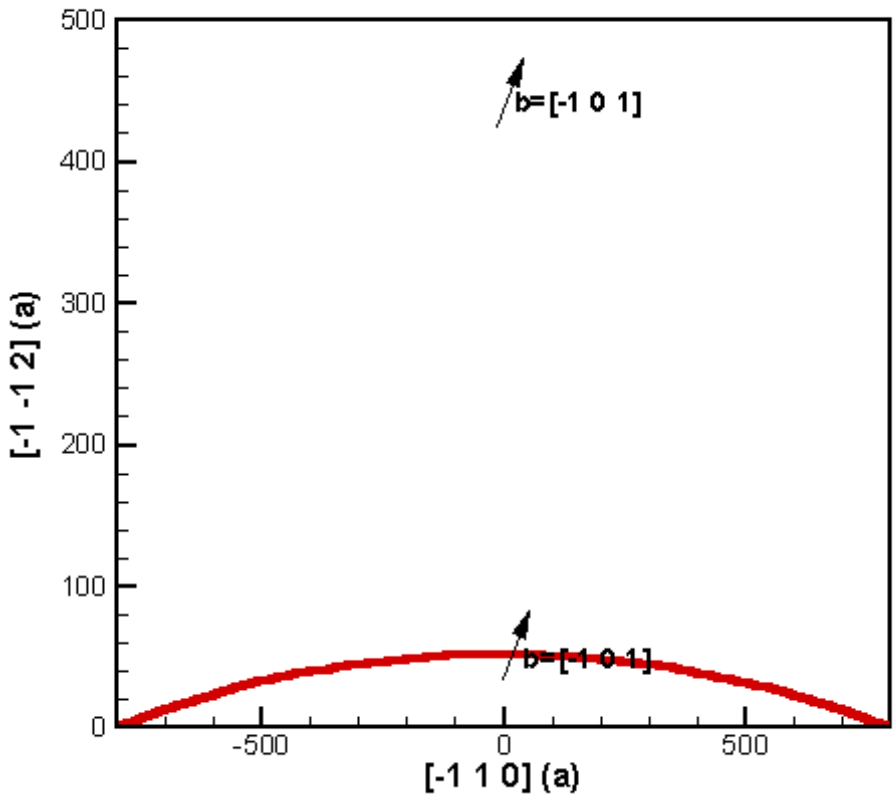
K=Mobility Matrix

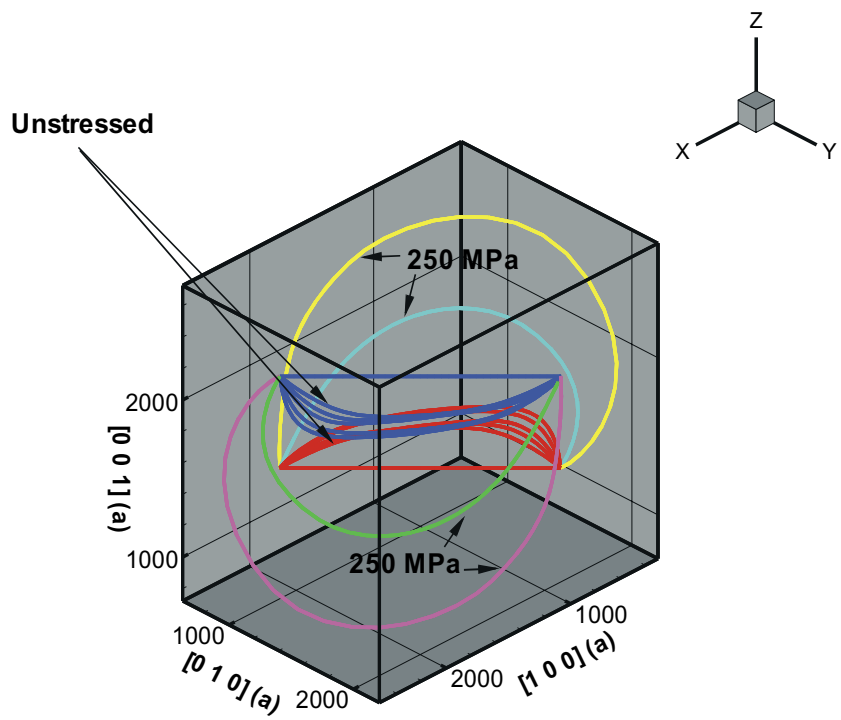
Node Redistribution



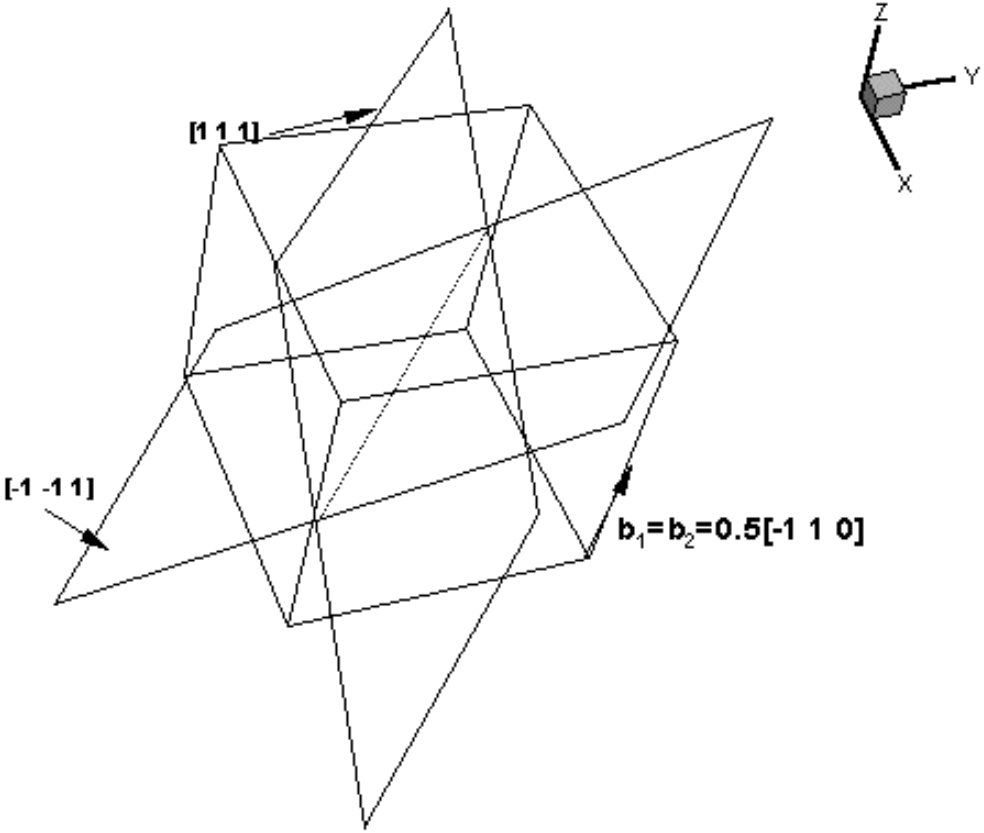


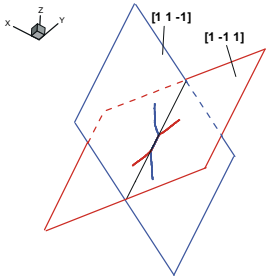
Formation and Breakup of Mixed Short Dipoles



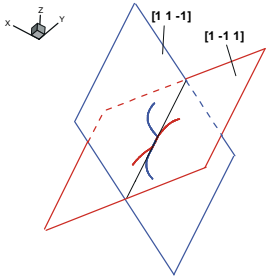


Formation and Breakup of a Junction

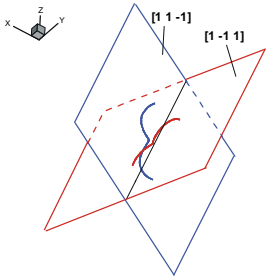




(a)

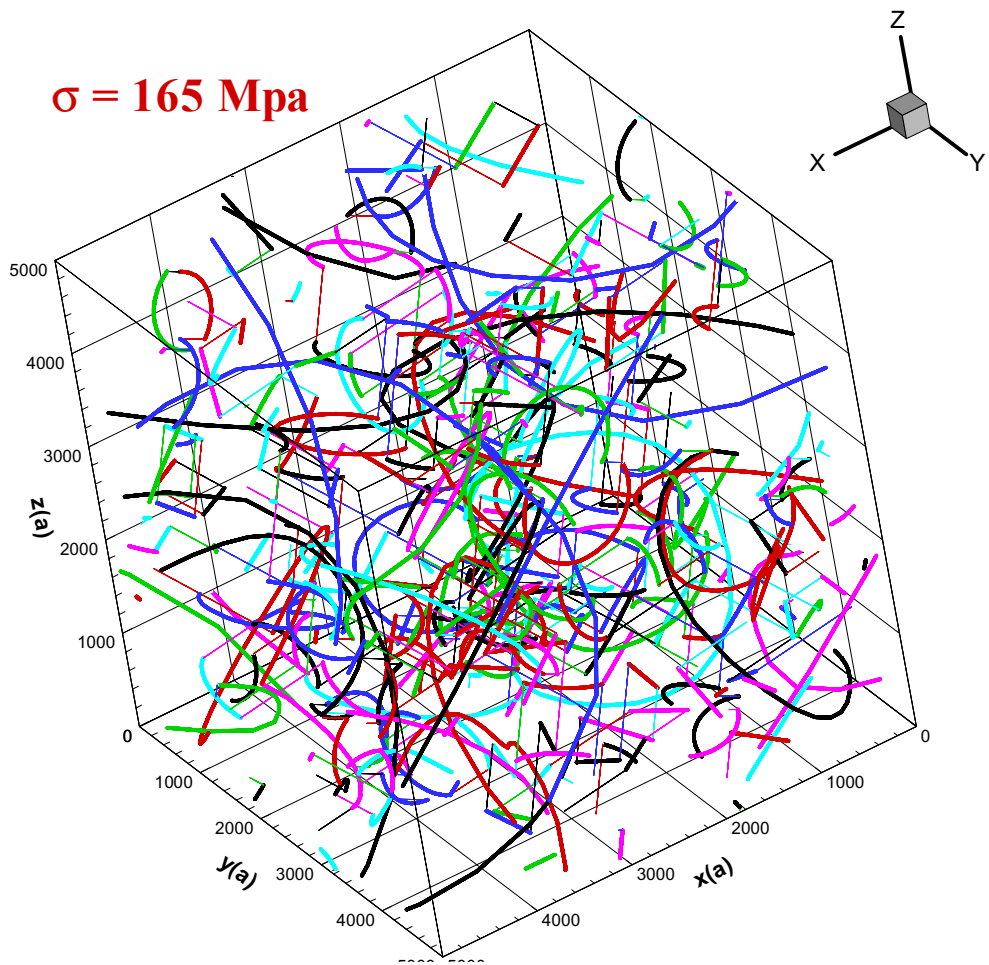


(b)



(c)

Large-Scale Simulation-2



Animation of Large-Scale Simulation

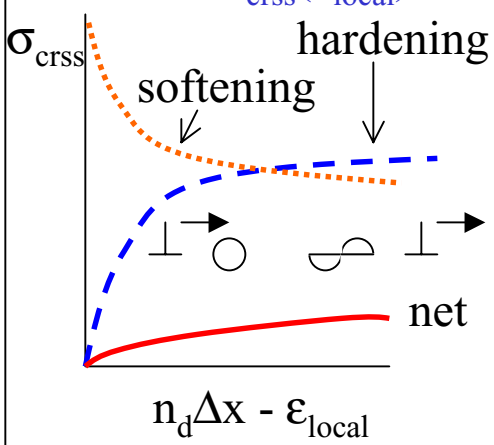
Shortcut to dynamic_deformation.lnk

Deconvoluting Localization Effects

- Isolate and properly integrate *multiscale* parts - and determine what controls observables

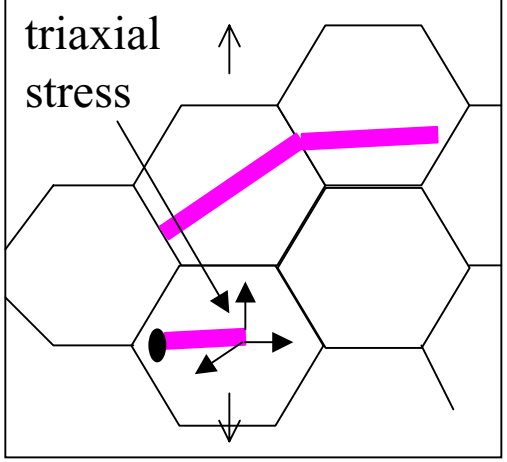
Microconstitutive

dislocation-obstacle interactions and processes controlling local $\sigma_{crss}(\varepsilon_{local})$



Micromechanics

deformation patterns and localization-depend on σ, σ-state redistribution

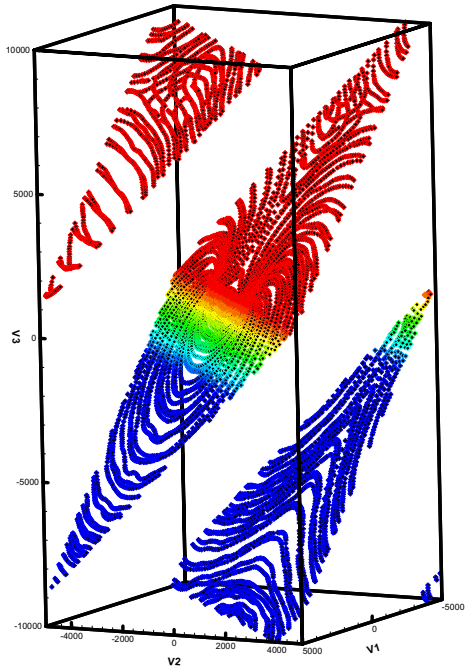


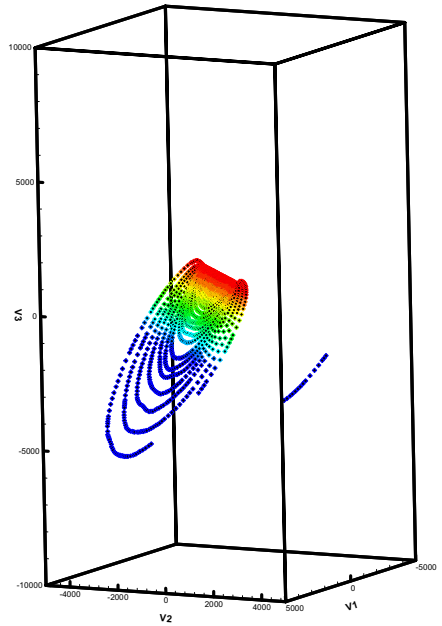
Continuum Mechanics

large geometry-change deformation and load-instability-necking

Single Slip Deformation – WSU – funded by ASCI/ LLNL

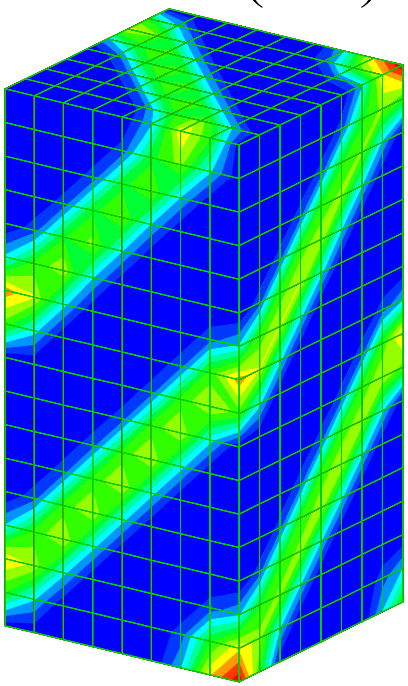
Elasto-plastic FEM DD Modeling of Localized Deformation Microshear bands

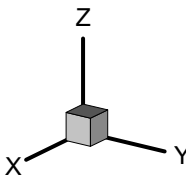




Dislocation path

(001)



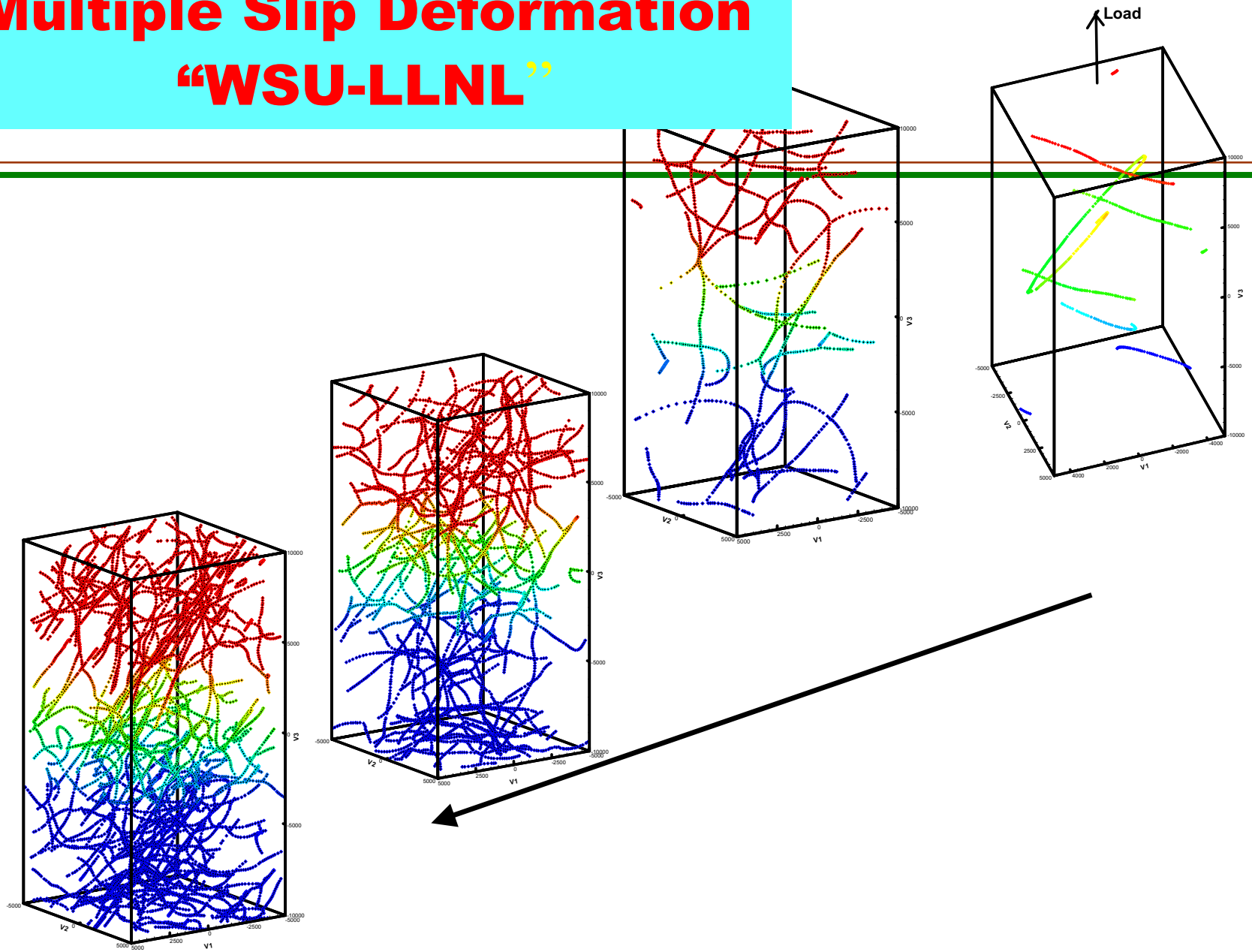


Effective Plastic Strain (

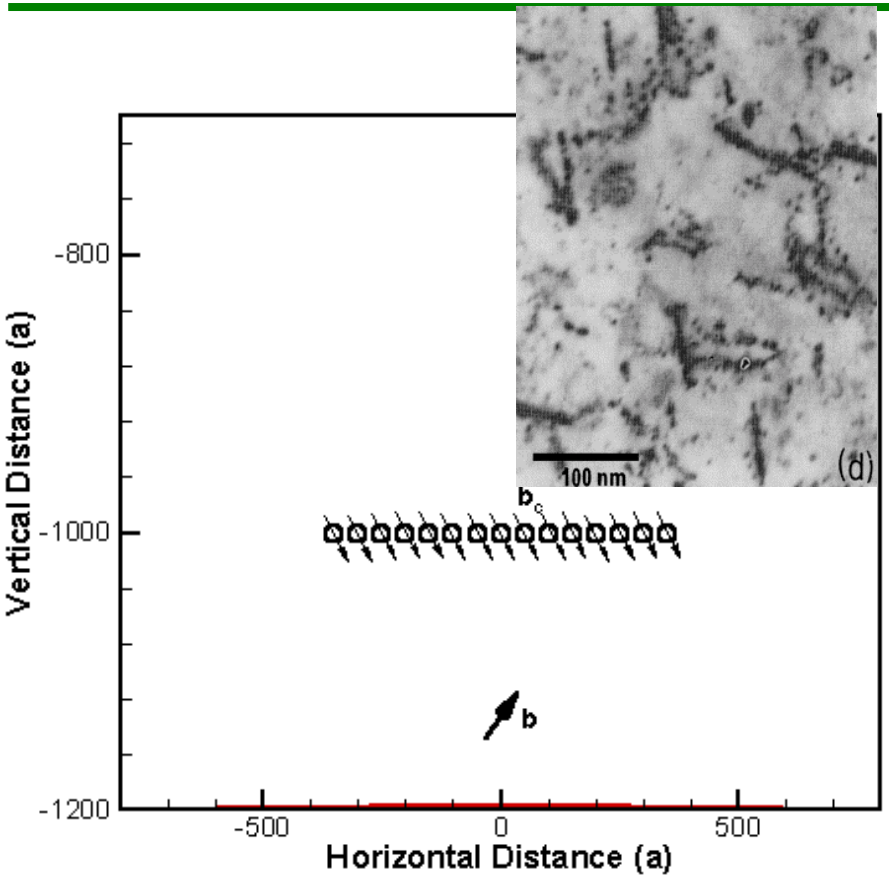
0.386407
0.270485
0.154563
0.0386407

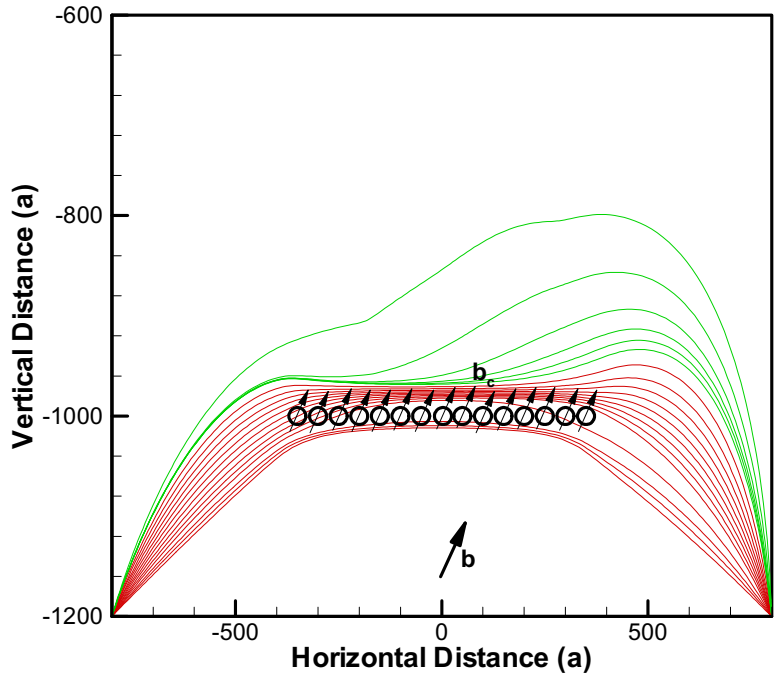
FCC: Periodic BC
Single Slip
One FR source

Multiple Slip Deformation "WSU-LLNL"



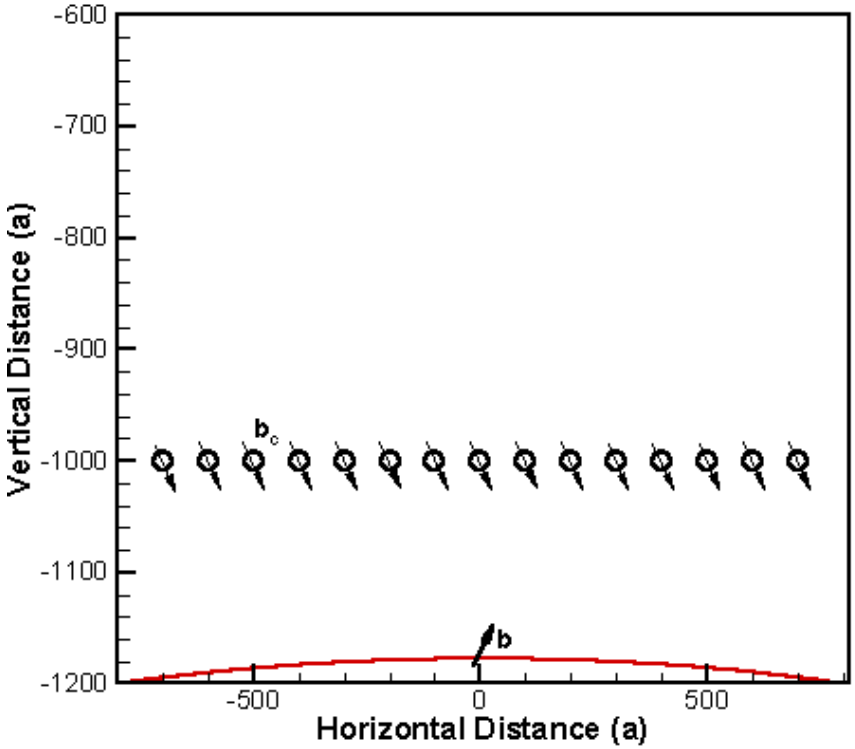
Mechanisms of Dislocation Unlocking from Cluster Atmospheres

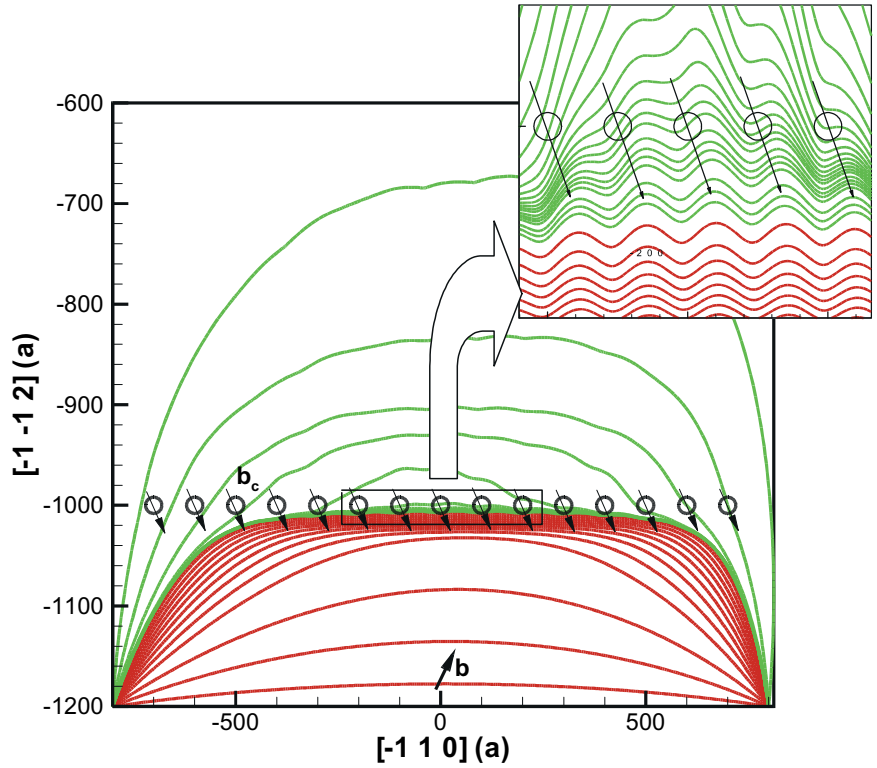




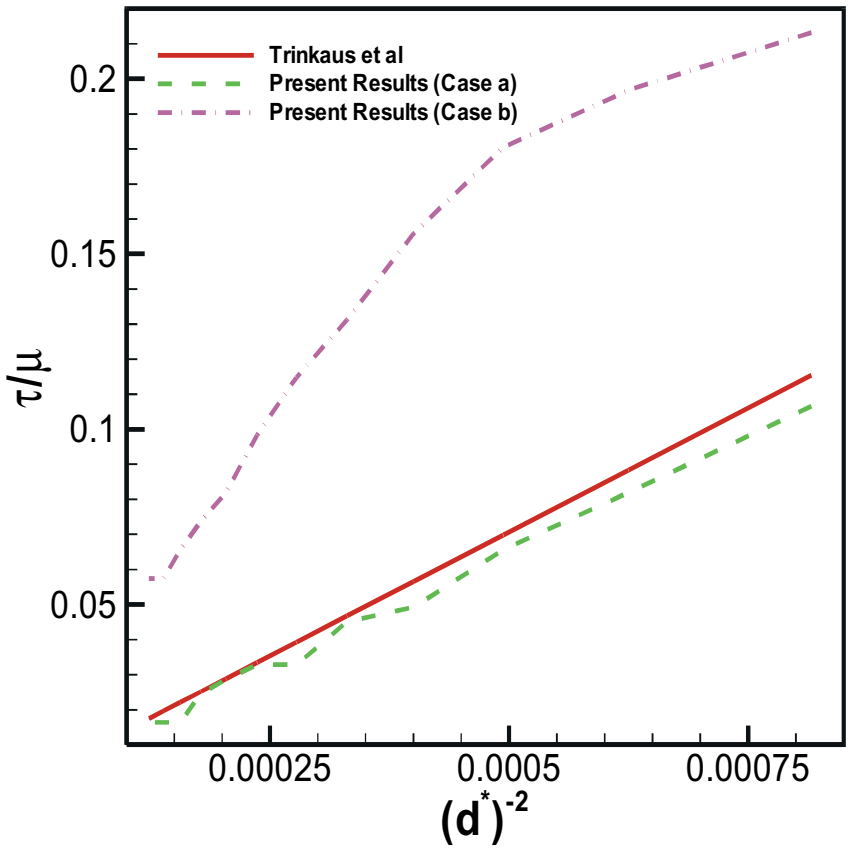
Z=D=40, L=50,b=1/2(-101),Stress = 200 MPa, Attractive Clusters

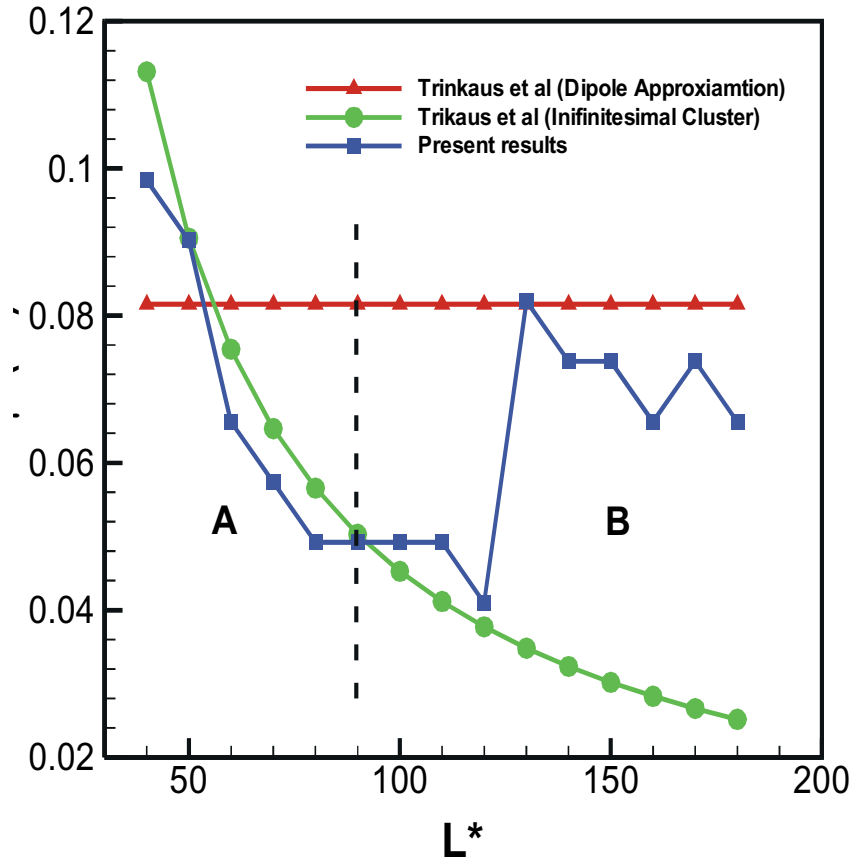
Symmetric Unlocking Instability



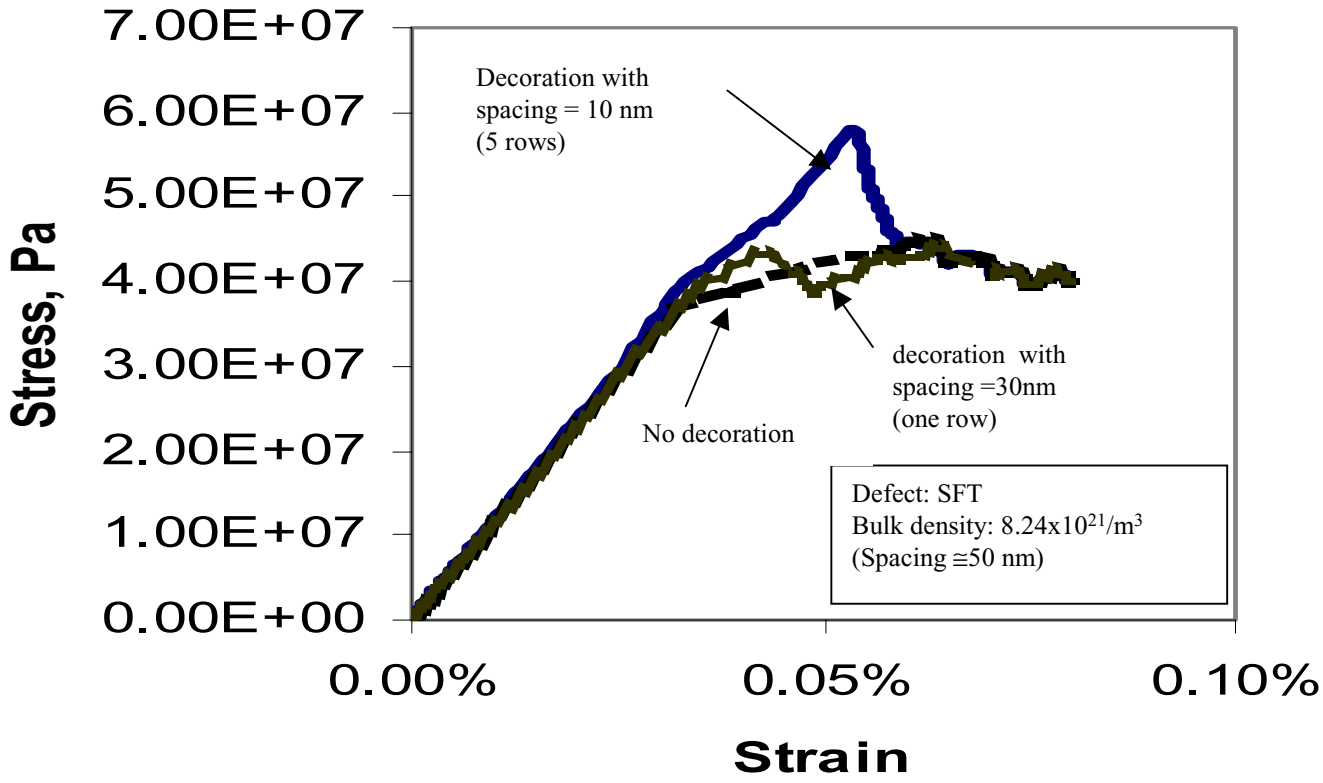


Flow Stress Scaling for Dislocation Unlocking from Cluster Atmospheres



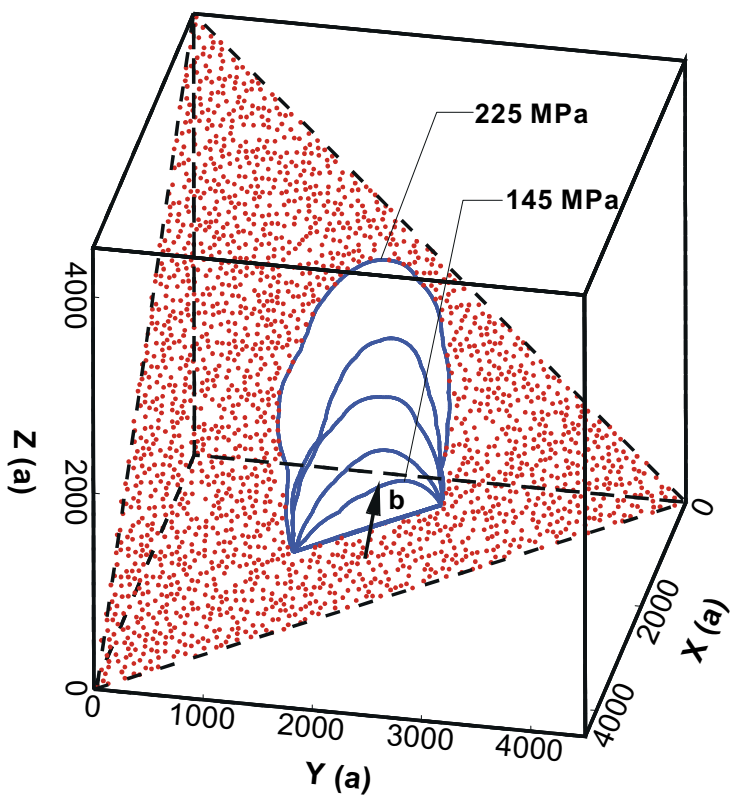


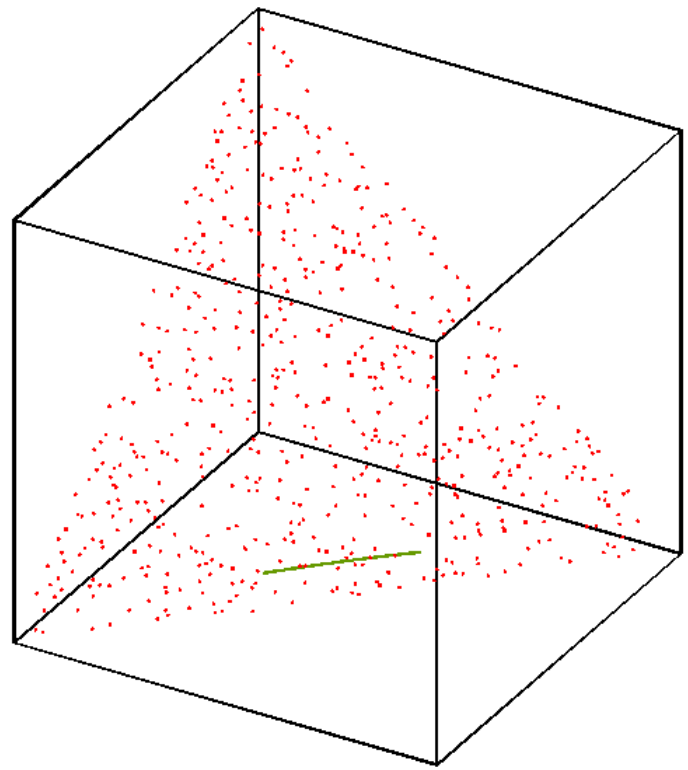
Stress-Strain Diagram in Pd "WSU-LLNL"



Yield drop is determined by "decoration density"
After drop, the flow stress is determined by the "bulk density" and "absorption" (free path)

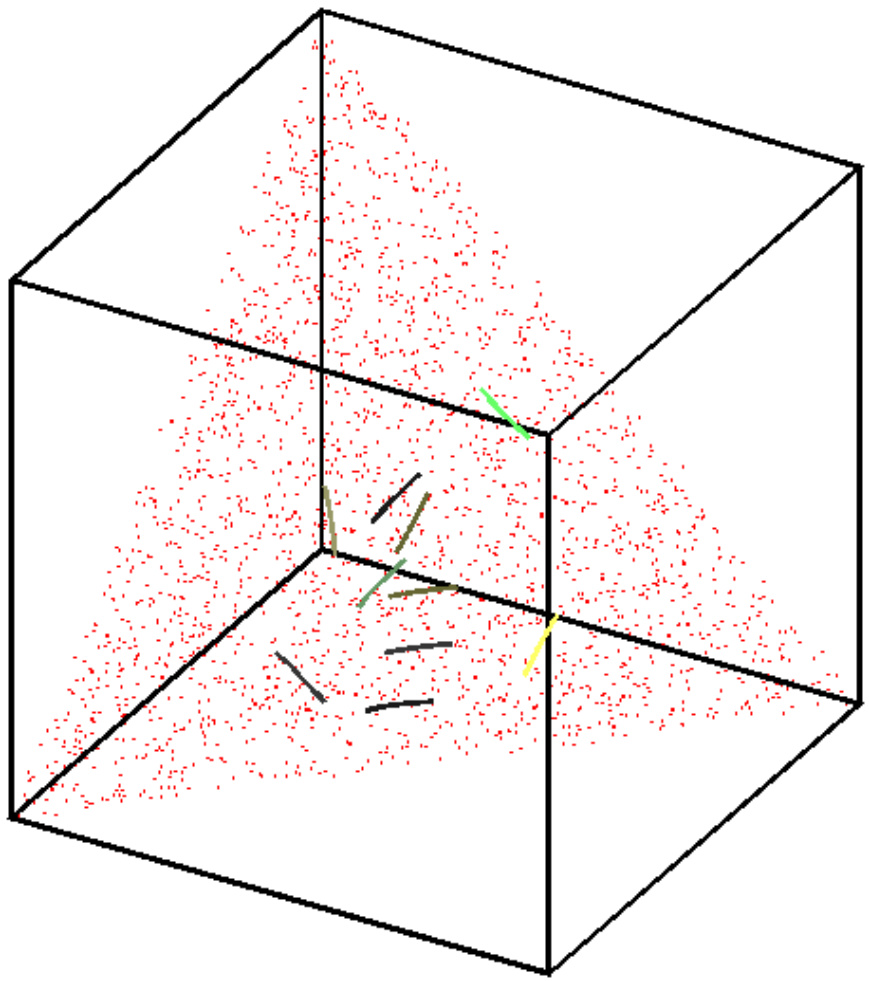
Applications to Flow Localization in Irradiated Copper



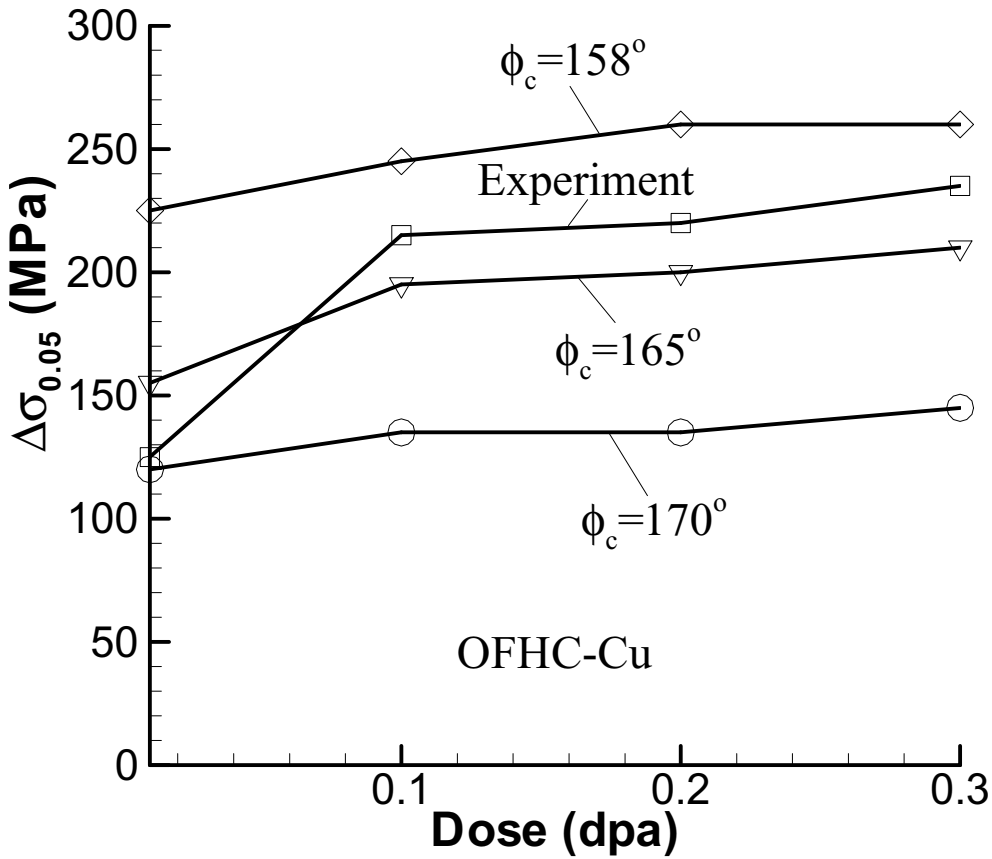


Dislocation glide results in destruction of Stacking Fault Tetrahedra and Climb

Evolution of Dislocation Channels



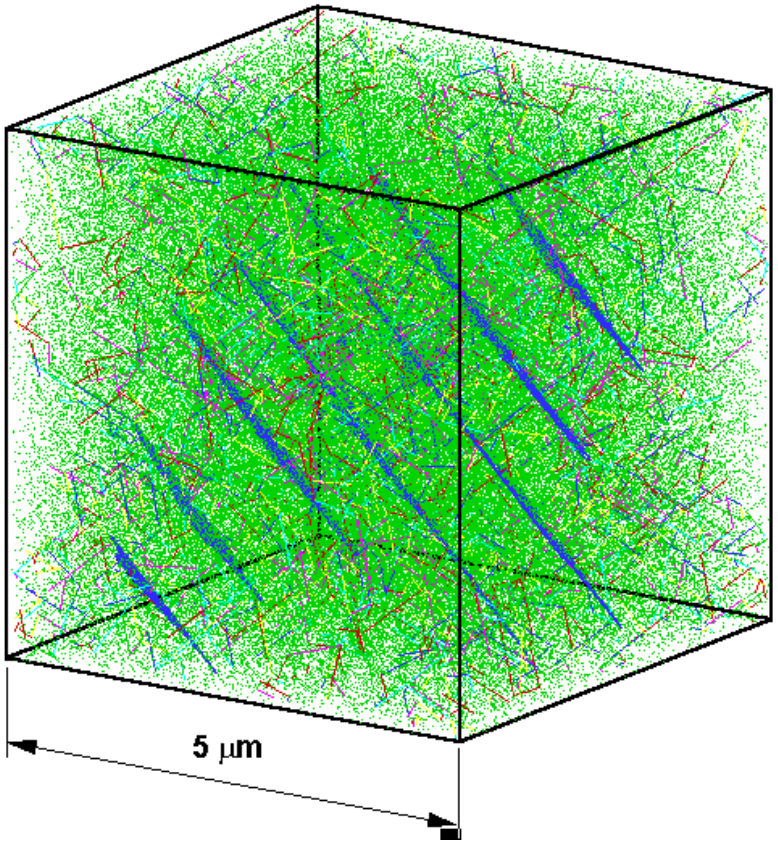
Comparison between Simulations and Experiment on Radiation Hardening in Cu



Comparison between Simulations and Experiment on Flow Localization

Experiment

Computer Simulation



Simulation of Dislocation Channels by Cross-slip "WSU-LLNL"

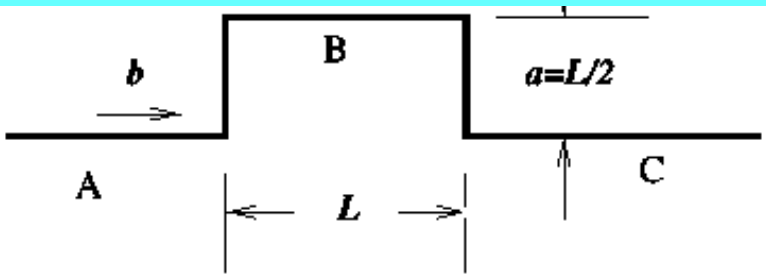


Figure 6.1 A bow-out "double-kink" model for cross-slip.

$$P = \alpha \frac{nC_t \delta t}{L} exp(-\frac{\Delta W^* - \tau A}{kT})$$

From frequency of vibrating dislocations segment of length L

$$\Delta G = \Delta W - \tau b A$$

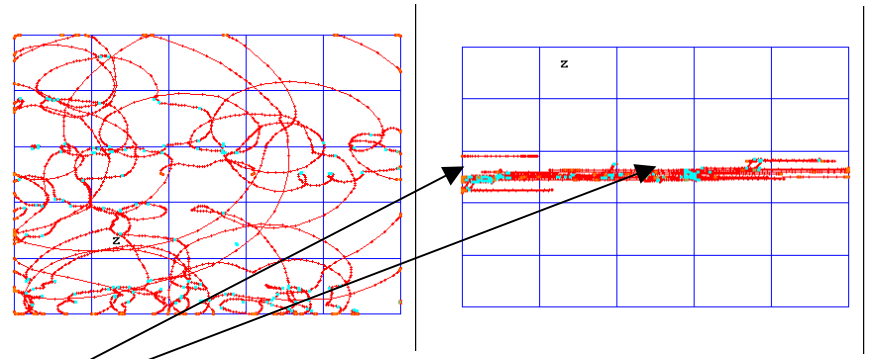
$$\Delta W = \frac{\mu b^2}{2\pi}\left[\sqrt{L^2+a^2} - L - a + L\,\ell n\left(\frac{2L}{L+\sqrt{L^2+a^2}}\right)\right]$$

$$-\frac{\mu b^2}{4\pi(1-\nu)}\left[2L - 2\sqrt{L^2+a^2} + 2a\,\ell n\left(\frac{a+\sqrt{L^2+a^2}}{L}\right)\right]$$

$$+\frac{\mu b^2 a}{2\pi(1-\nu)}\ell n\left(\frac{a}{e\rho}\right)$$

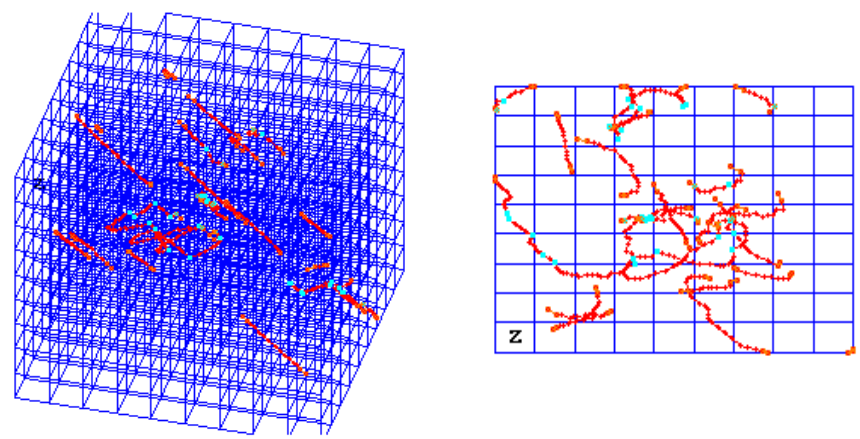
Top view [111]

Side view [1,-1,0]

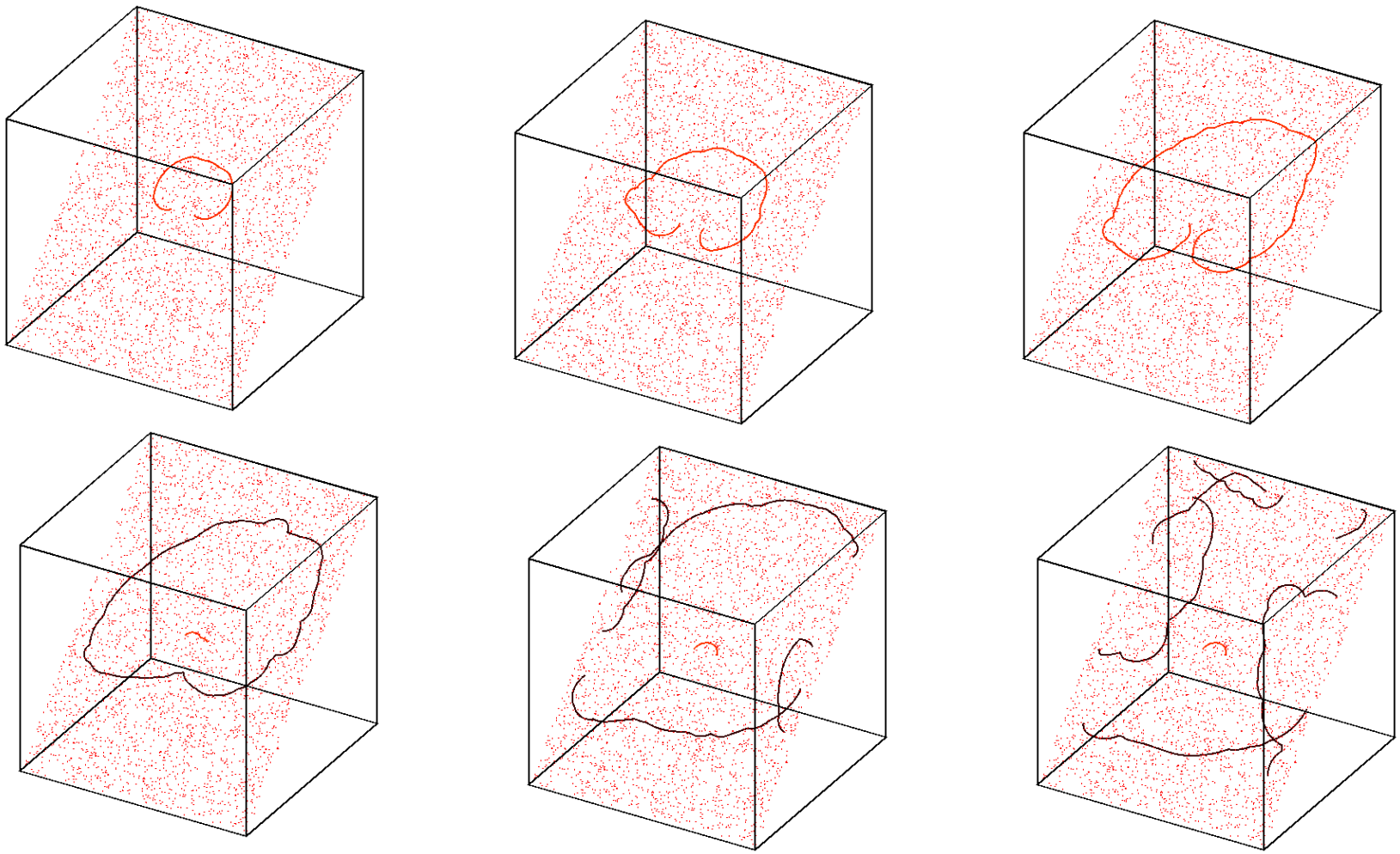


Spreading of a single FK sources by cross-slip

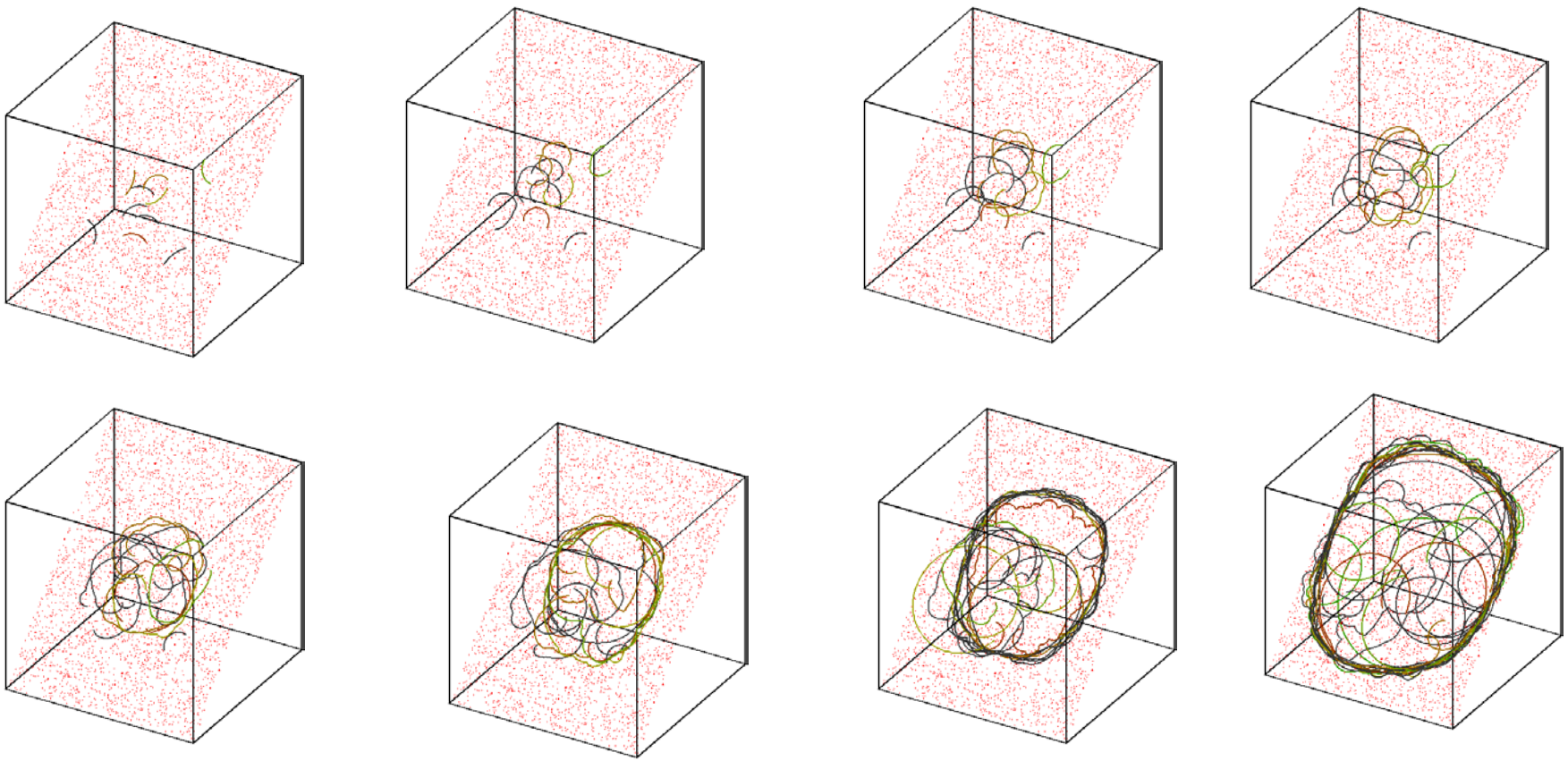
Double cross-slip



Evolution of Dislocation Channels in Fe Single FR-source



Evolution of Dislocation Channels in Fe Multiple FR-sources



Dislocation glide results in destruction of micro-voids and climb

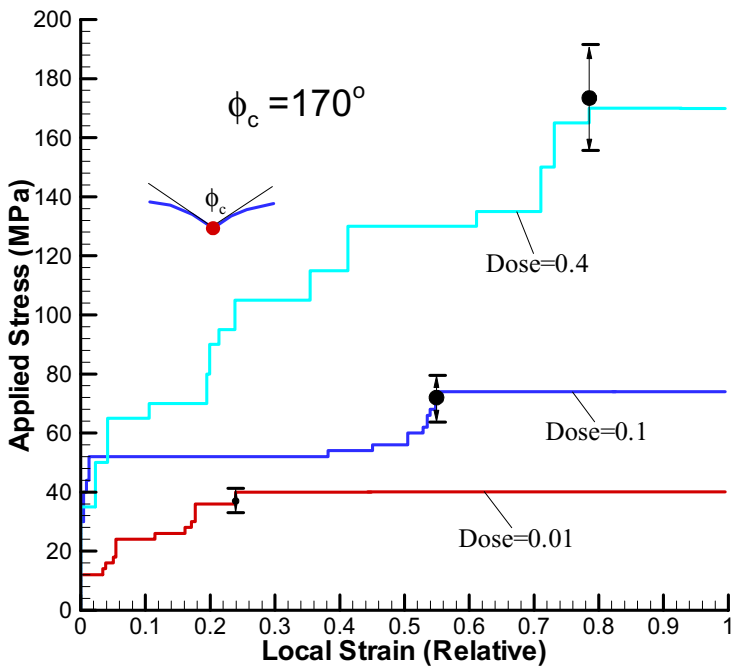
Evolution of Dislocation Channels in Fe – Animation

Shortcut to bcc1.lnk

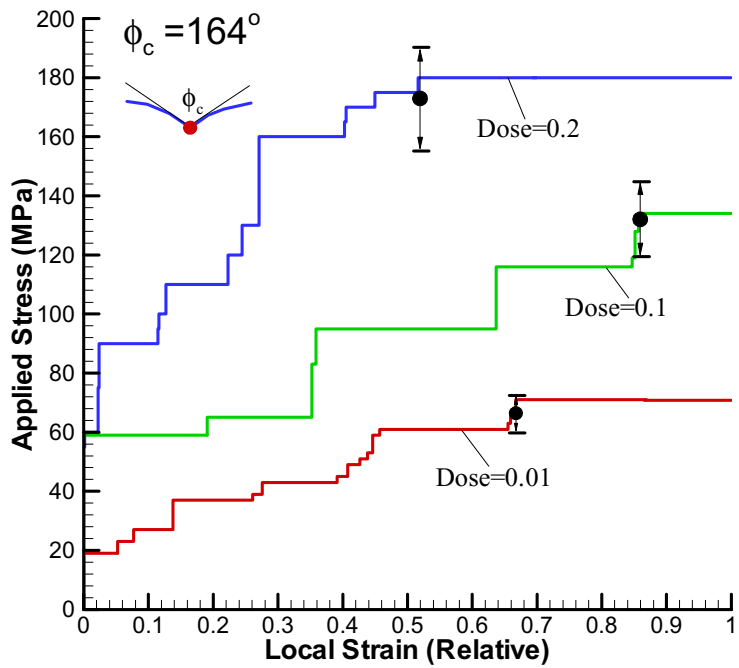
Shortcut to bcc_mul3.lnk

Shortcut to bcc_mul_side.lnk

Comparison between Simulations and Experiment on Radiation Hardening in Fe-1

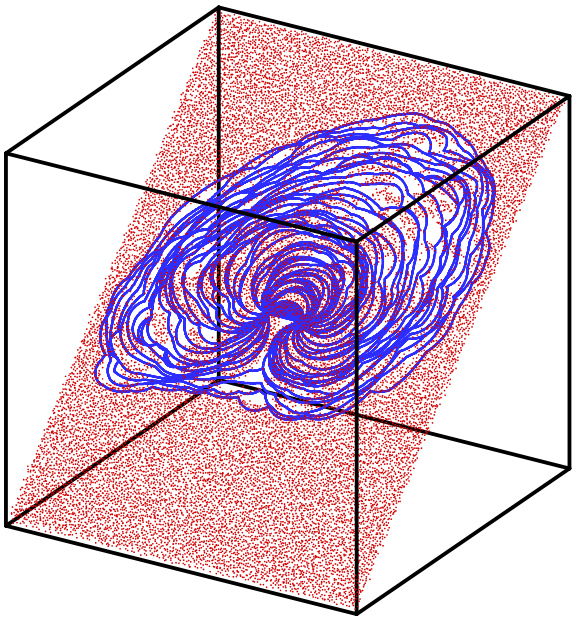


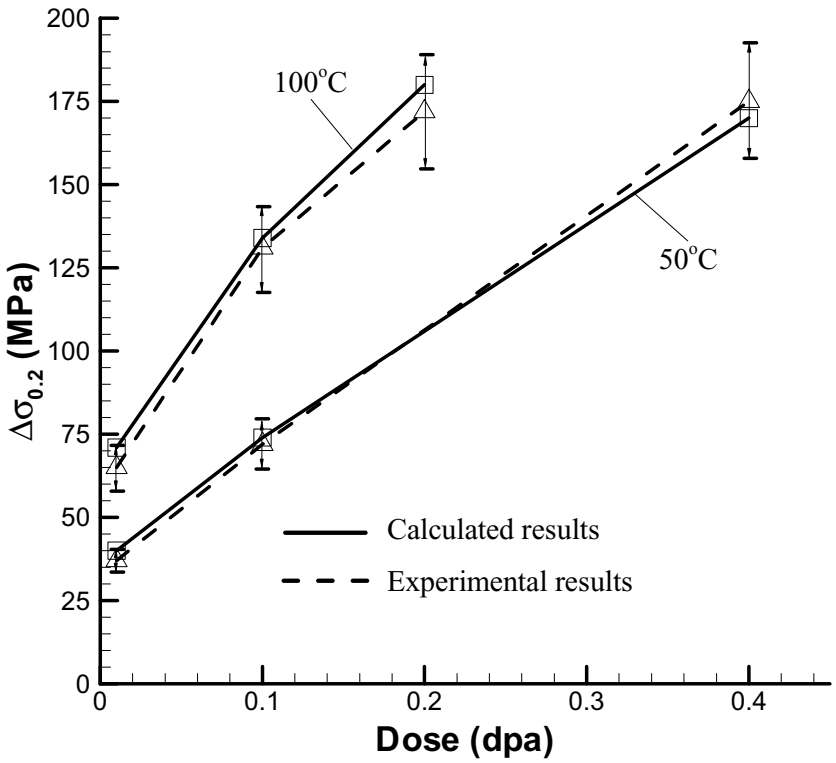
50 ^{O}C



100 ^{O}C

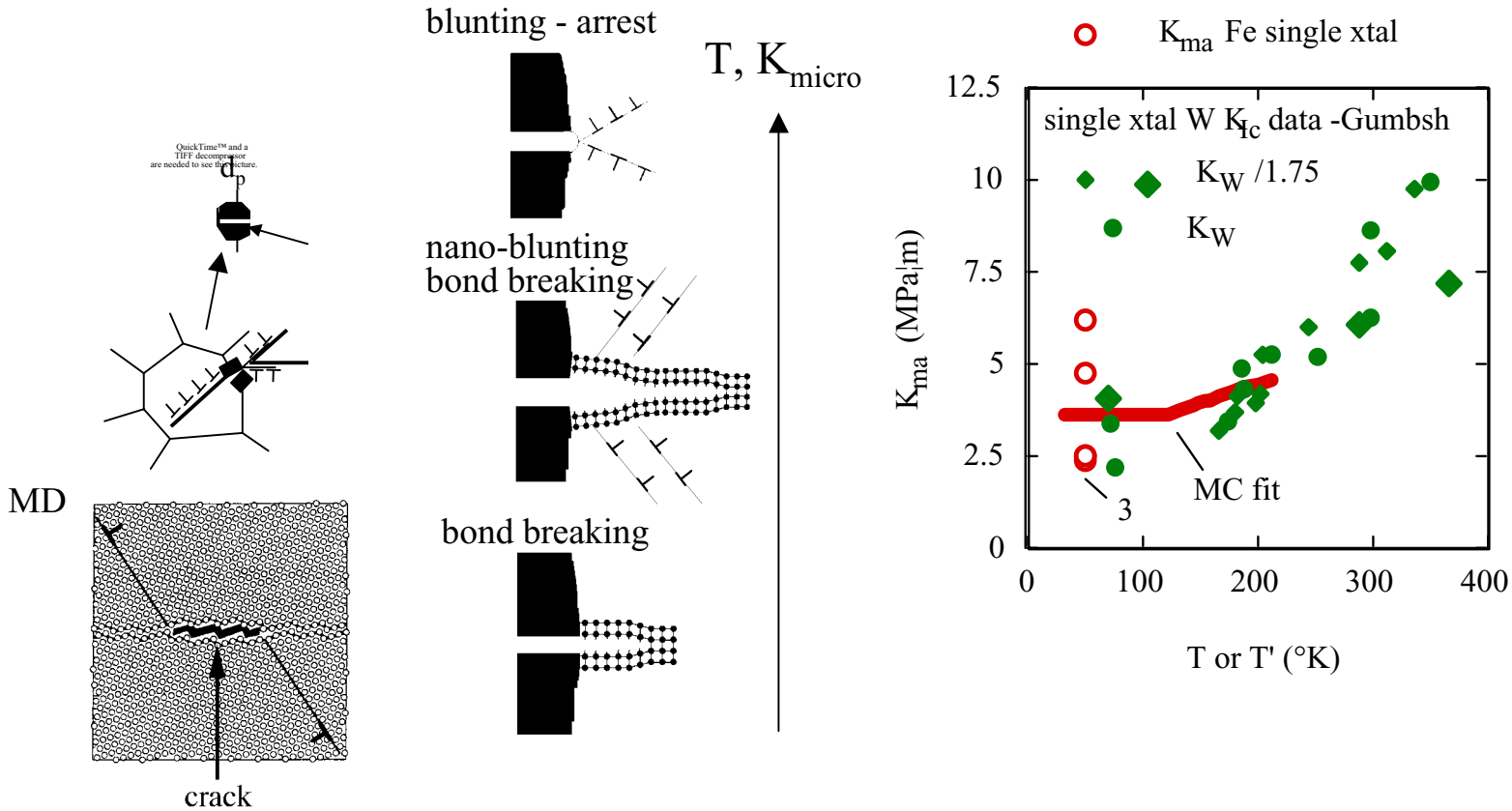
Comparison between Simulations and Experiment on Radiation Hardening in Fe-2





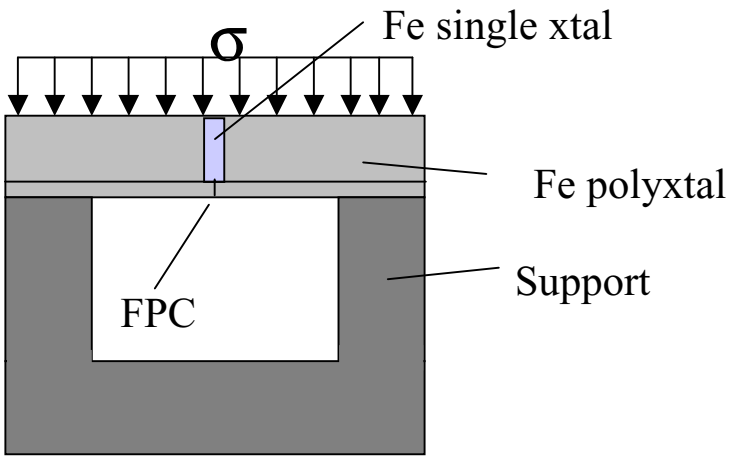
$K_{ma}(T)$

- **The $\sigma^*(T) \approx C_g K_{ma}(T)/\sqrt{d_p}$ -- postulate that $K_{ma}(T)$ controlled by dynamic microcrack tip dislocation processes inherent to Peierl's stress of a bcc lattice**

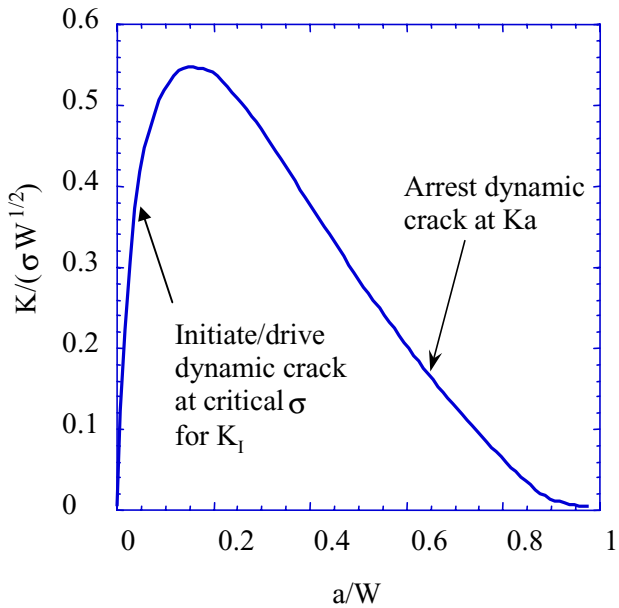


Experiments to Measure $K_{ma}(T)$

- **Measure K_a in oriented (100)[010] Fe single xtals using special composite specimens in compression anvil fixture.**
- **5 tests to date at -198°C K_a = 3.7±1.7 MPa√m**



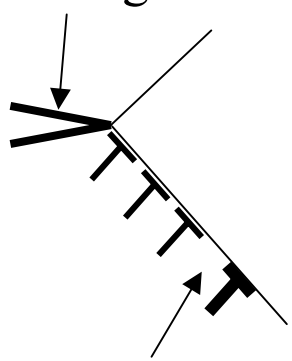
diffusion bond: single/3 polyxtal Fe, FPC, machine to proper a/W

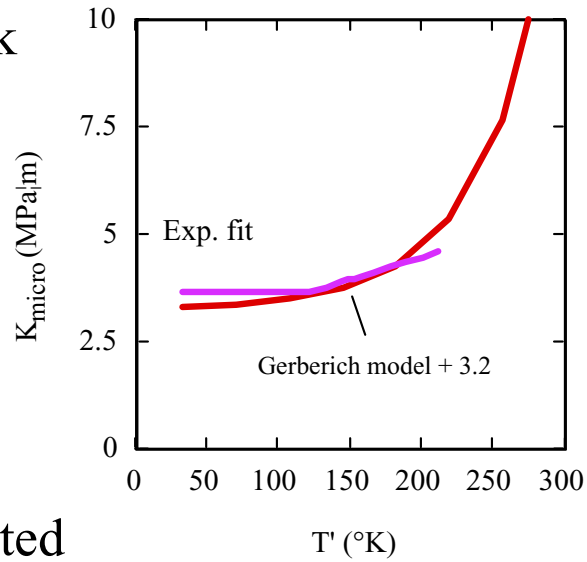


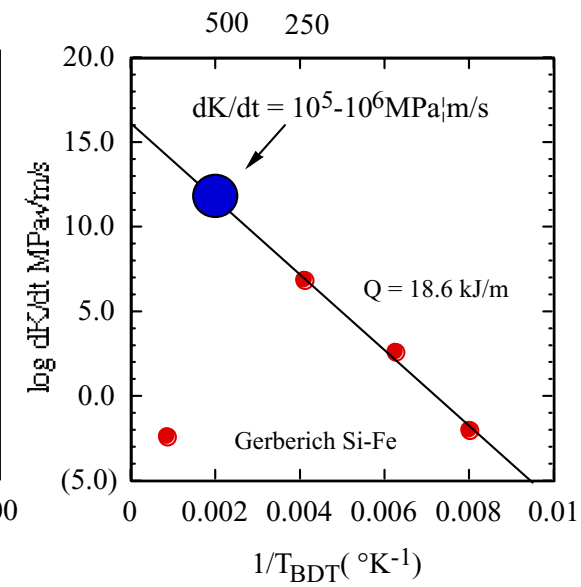
Modeling $K_{ma}(T)$

- **Modify Gerberich (super) dislocation shielding model to account for higher Peierl's stress under dynamic microcrack loading conditions.**

Running microcrack







Shielding by array of superdislocations limited by velocity dependent lattice mobility.

Conclusions and Future Directions

- Dislocation Dynamics (DD) is shown to be a very useful tool for accurate simulation of mesoscopic plastic deformation of irradiated materials.
- Detailed conditions for the majority of dislocation interactions have been worked out (e.g. dipoles, junctions, cluster interaction, etc.).
- New mechanisms for dislocation unlocking from cluster atmospheres are uncovered.
- The basic mechanism of flow localization in irradiated materials is demonstrated by computer simulations.
- Good agreement between simulations and experiment on hardening.
- <u>Future Research:</u>
  - DBTT in unirradiated and irradiated Fe and V.
  - Effects of alloying on plastic flow localization.
  - Coupling between mesoscopic DD and macroscopic FEM.