Defect Obstacle Interactions and Microstructure-Hardening Models

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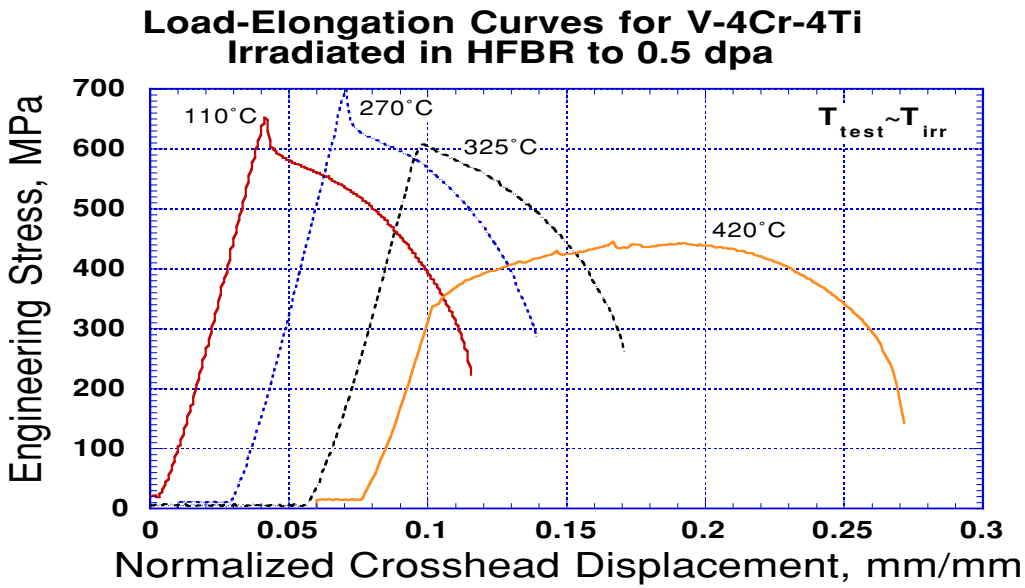
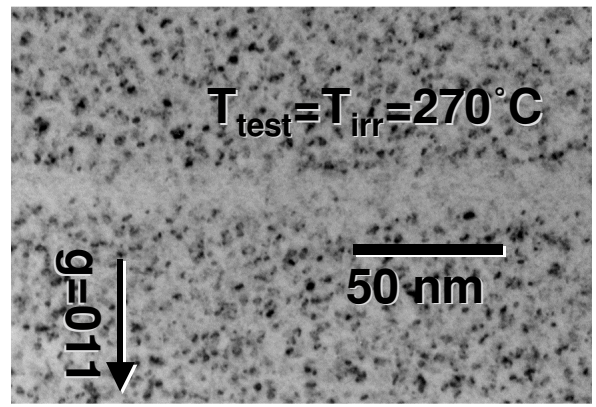
Introduction and objectives



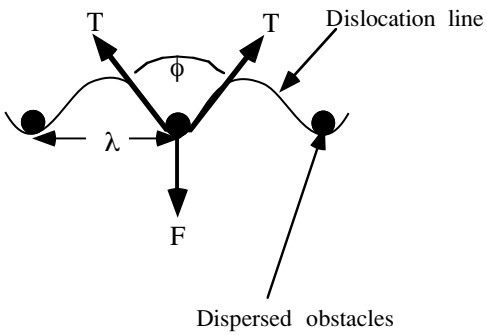
Radiation defects & microstructures



- Review current state of understanding and look forward
  - Dispersed barrier hardening and cascade induced source hardening
  - Microstructure observations, yield stress changes and α-values
  - Atomistic (MD) simulations of defect - obstacle interactions
  - Constitutive modeling

Dispersed barrier hardening

- Radiation obstacles (loops, voids, SFTs, precipitates, etc…) typically treated as dispersed barrier obstacles -implemented in yield stress ($\Delta\sigma_y$)



$$\sigma_{obs} = \alpha \frac{M\mu b}{\lambda} \cos\left(\frac{\phi_c}{2}\right) \qquad \lambda \sim 1/\sqrt{Nd} \qquad \sigma_{obs} = \alpha' M\mu b\sqrt{Nd}$$

$$\Delta\sigma_y = \left[\sum_i \left(\alpha'(i) M\mu b\sqrt{N(i)d(i)}\right)^2\right]^{1/2}$$

- Traditional approach - microstructural examinations to determine N, d of radiation obstacles - relate to observed $\Delta\sigma_y$ to fit effective α' based on given superposition law - typical values of α' range from 0.1 (small vacancy clusters) to 0.3 (interstitial loops)

- Outstanding issues - Predictions of post-yield flow behavior, yield drop, obstacle features not observed in TEM, atomistic models of α'

Cascade induced source hardening

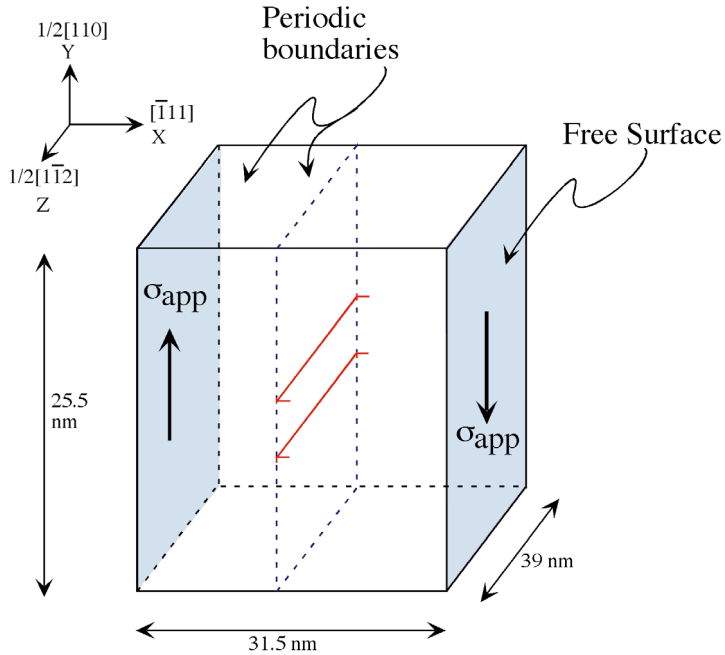
- Microstructural observations (dislocation loop rafting and decoration of dislocations) + observed yield drop in tensile tests led to the cascade induced source hardening model

- Outstanding issues
- CISH does not agree with PIA yield strength increases (Edwards), ignores matrix hardening
- in-situ TEM deformation observations (Robach & Robertson) show channel initiation from grain boundary and stress concentrated sources, not pre-existing matrix dislocations
- Prediction of post-yield deformation

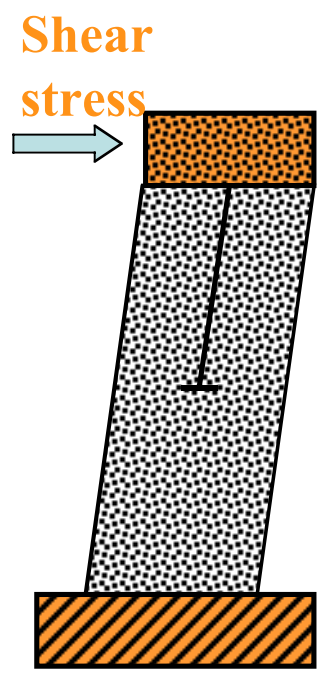
Atomistic simulations of dislocation - obstacle interactions

- Molecular dynamics (MD) simulations - introduce dislocations and radiation obstacles, equilibrate at temperature based on EAM/F-S interatomic potentials and apply constant stress (strain rate)

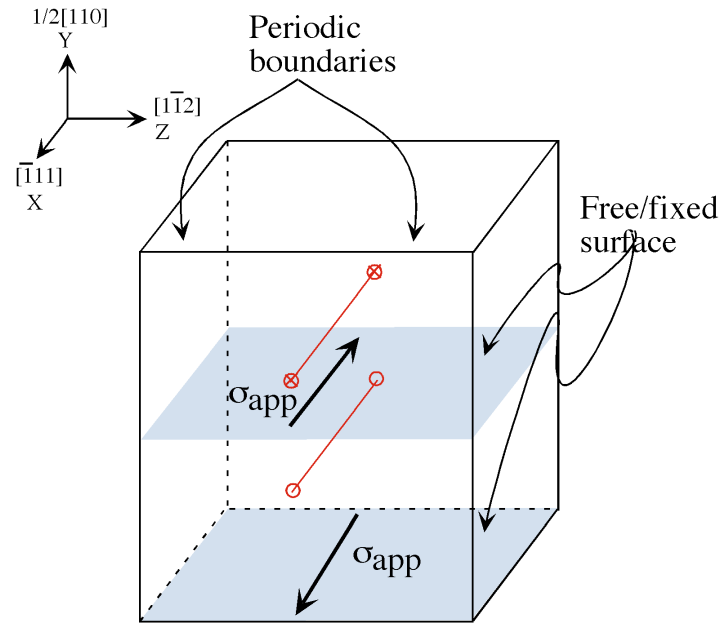
Edge dislocation - (Livermore)



Edge dislocation - (Liverpool)



Screw dislocation - (Livermore)

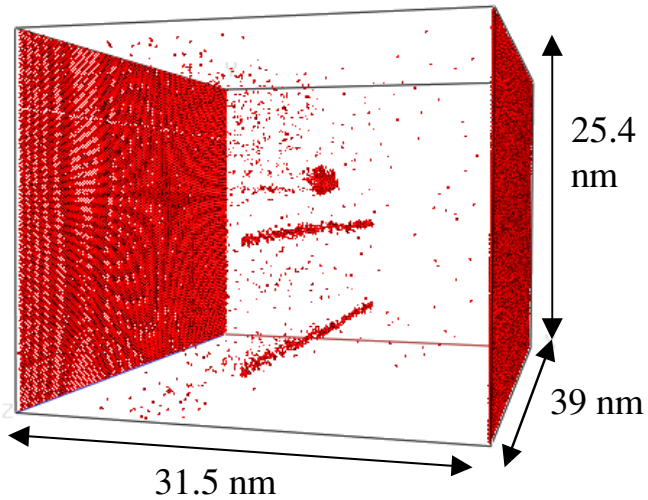


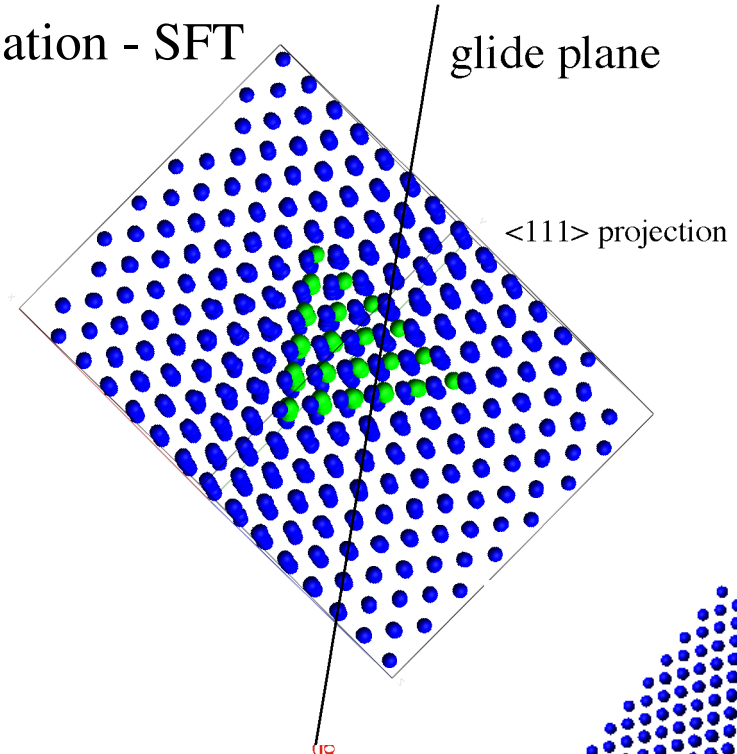
Insert screw dipole, slice off 1/2 of cell

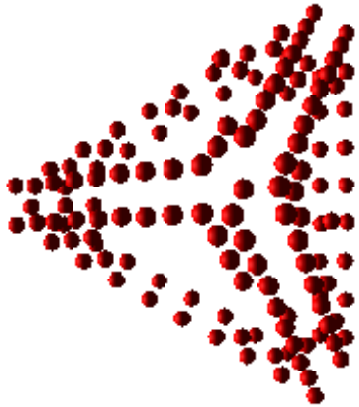
- Practical limitations
  - MD: high strain rate interactions, periodic boundary conditions - dislocation arrays
  - MS: static (equilibrium) structures, F-ΔX relationships

Edge dislocation - SFT, truncated SFT interaction

- Edge dislocation - SFT

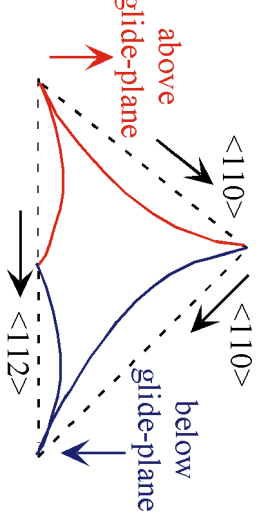


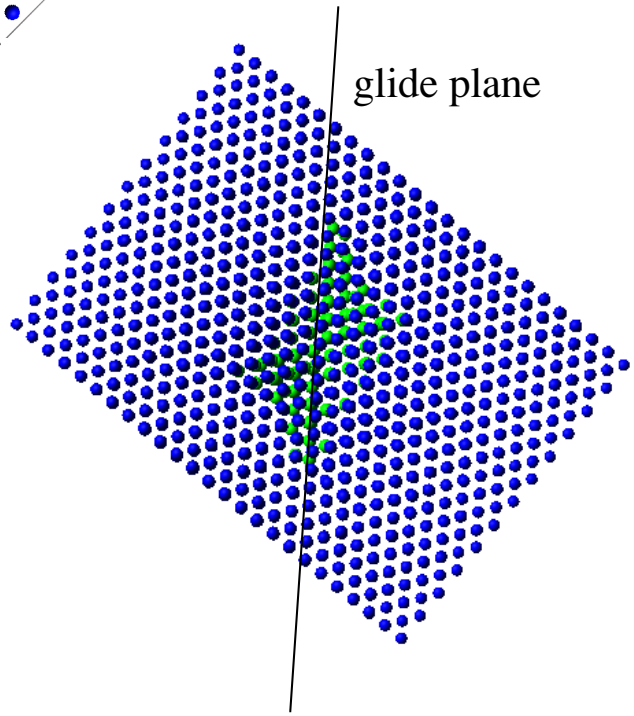




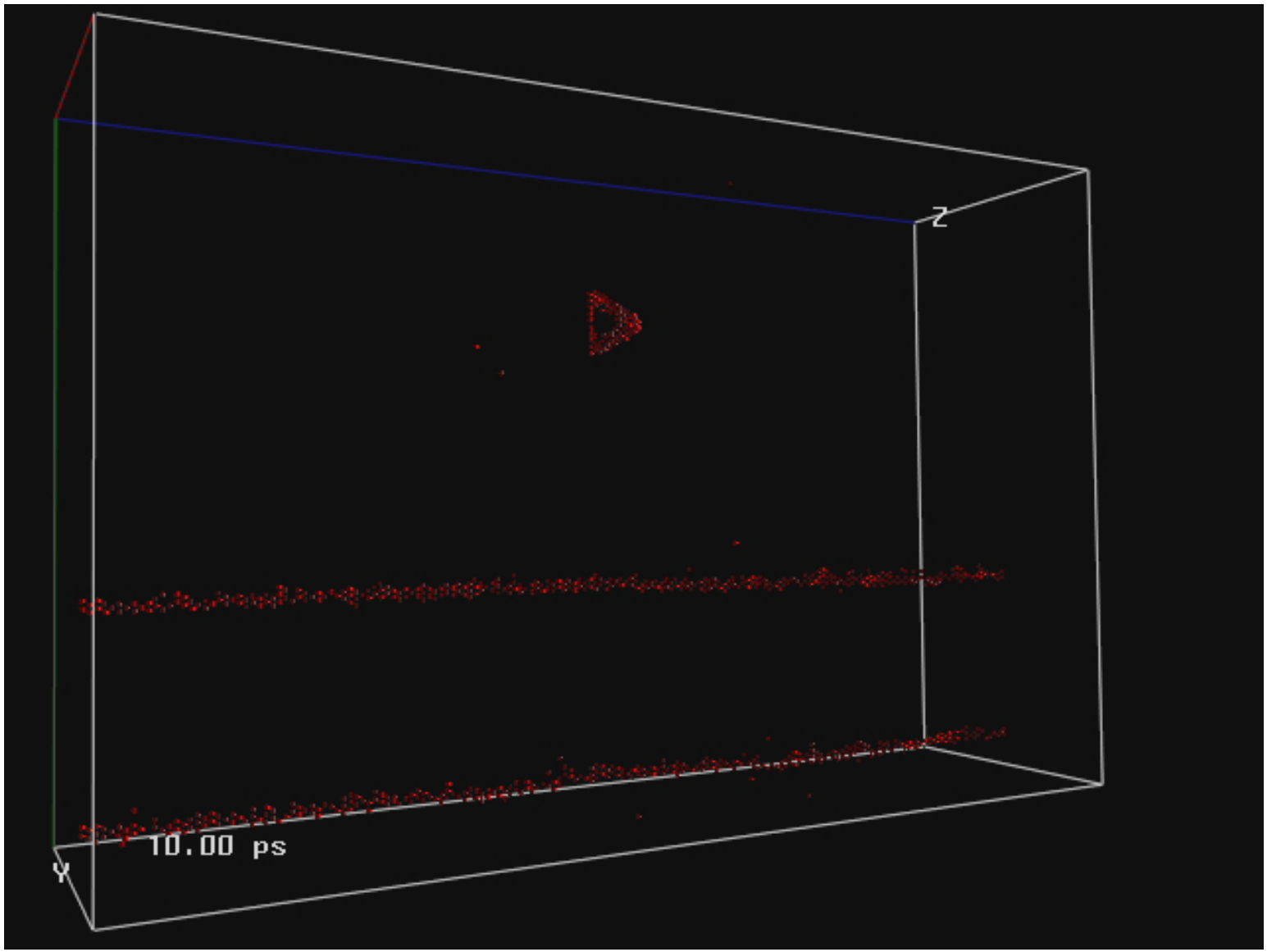
- Visualization by atoms with high potential energy

- Edge dislocation - overlapping, truncated SFT





Dislocation - SFT interaction in Cu (300 MPa)



Dislocation - SFT interaction movie

near - <111> projection

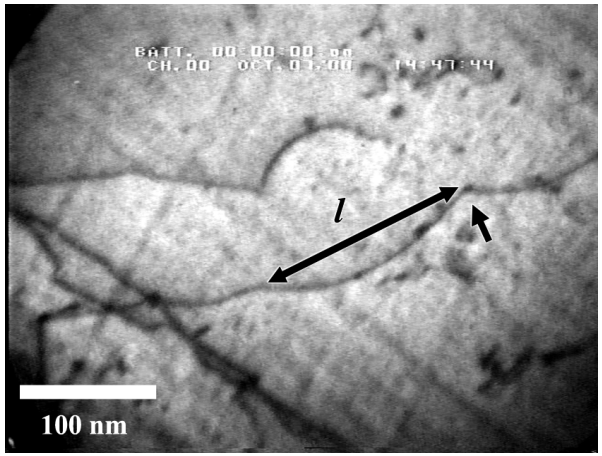
- SFT is a relatively strong obstacle $\phi \sim 80°$

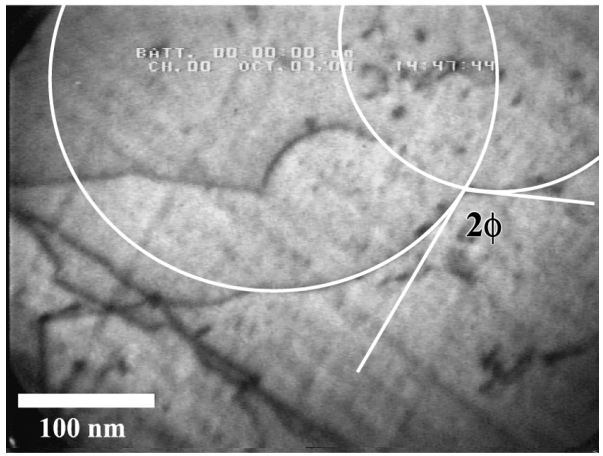
- SFT sheared but neither absorbed or destroyed

Dislocation - overlapping, truncated SFT in Cu (300 MPa)

- OTSFT absorbed, leading to super-jog pairs - re-emmitted as dislocation loop (a/2<110>) and subsequently re-absorbed, dragged and re-emmitted

Dispersed barrier hardening - obstacle strengths

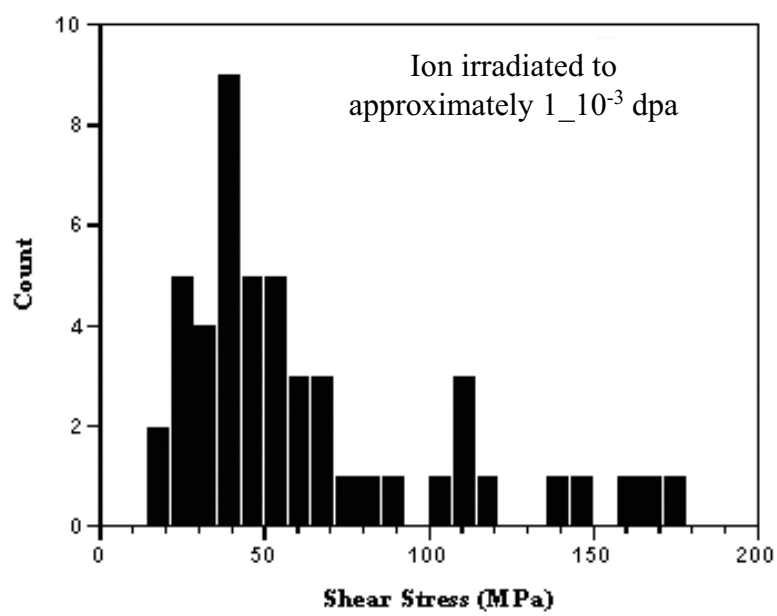




$$\tau = \frac{Gb}{l}(\cos\phi_c)^{\frac{3}{2}}$$

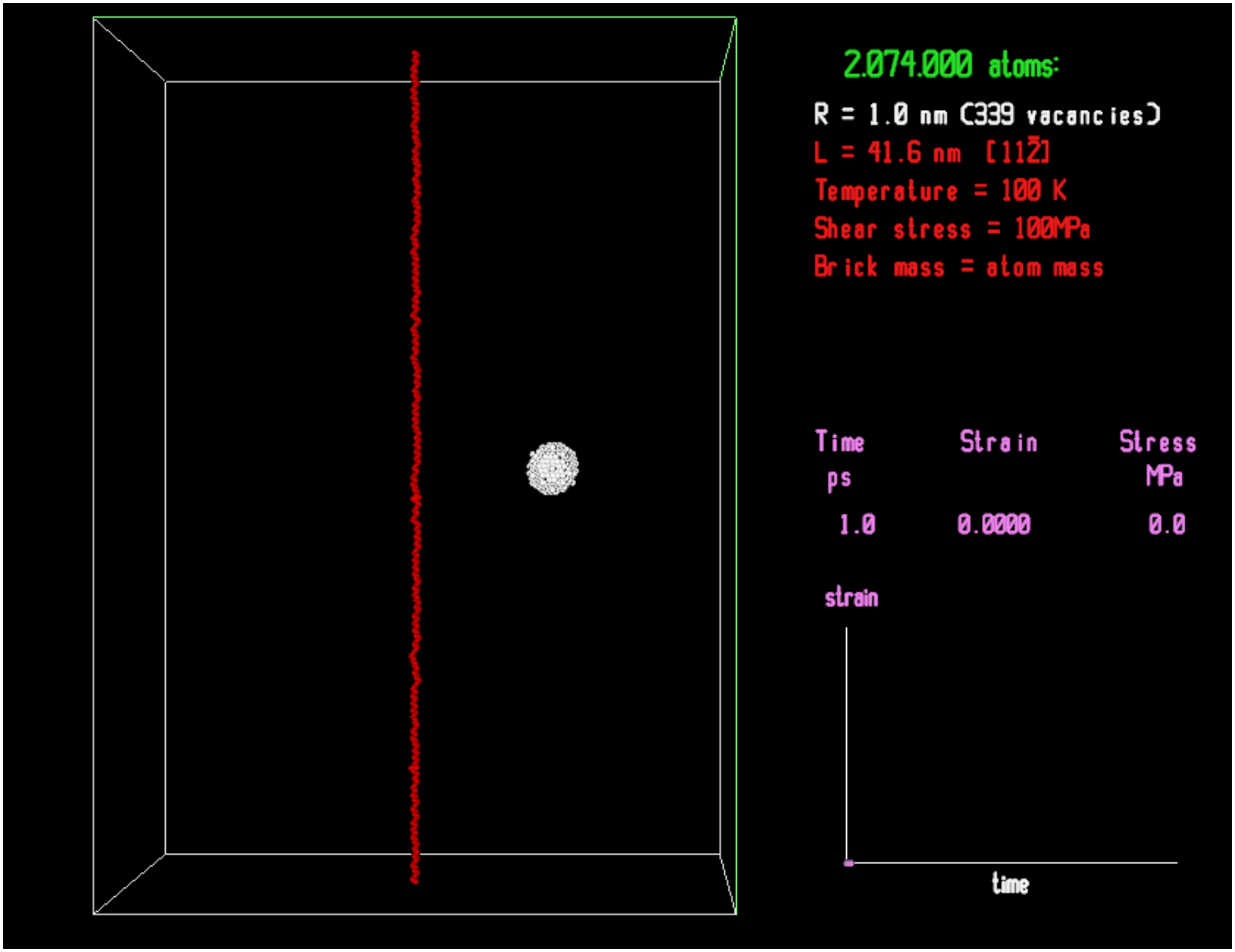
Fleischer-Friedel expression of the dispersed barrier hardening model

The local critical shear stresses determined from input of measurements into DBH theory are centered around 40 MPa. Yet, higher values are possible.



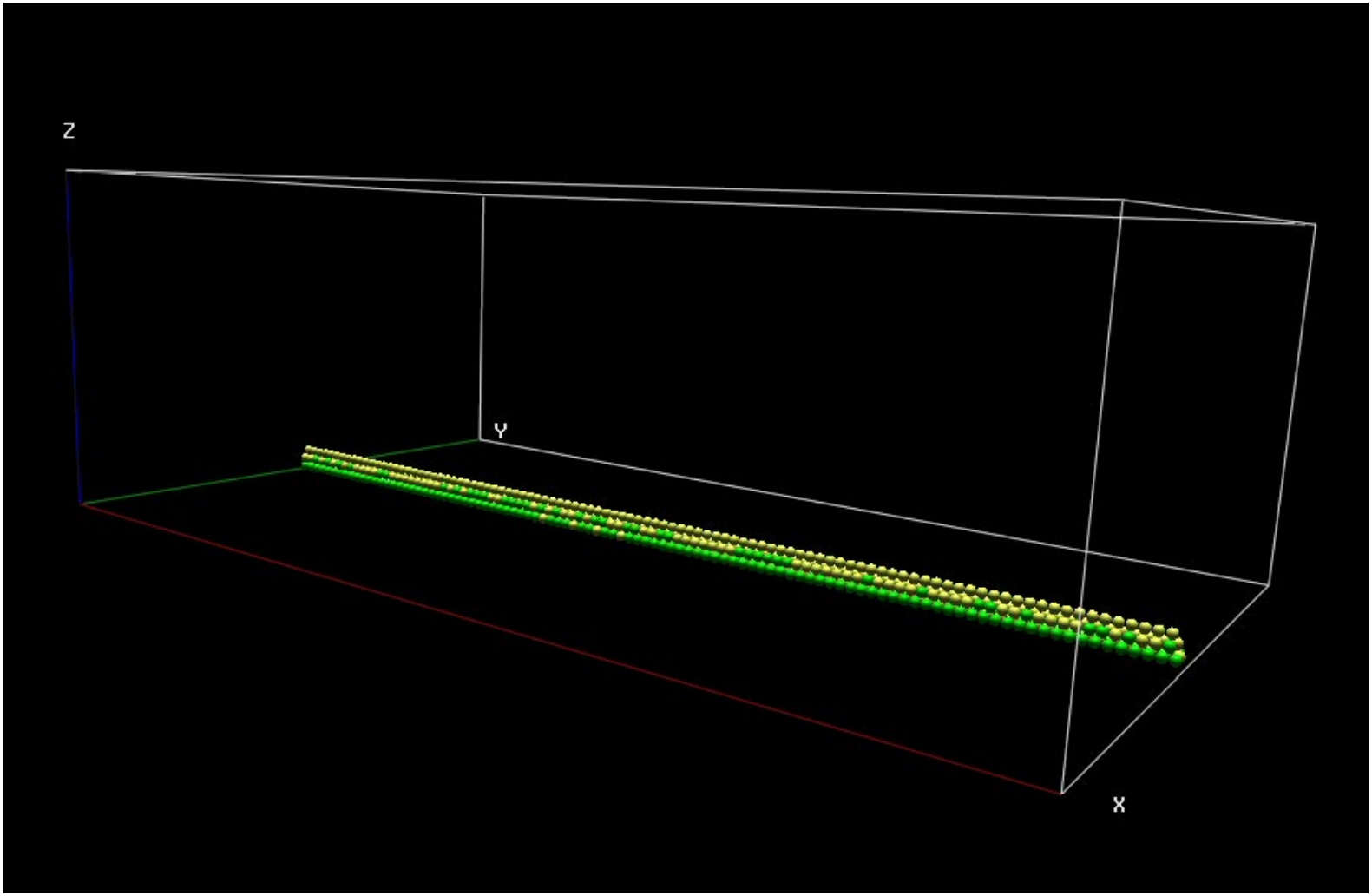
J. Robach and I. Robertson

Dislocation - void interaction in α-Fe (~ 100 MPa)



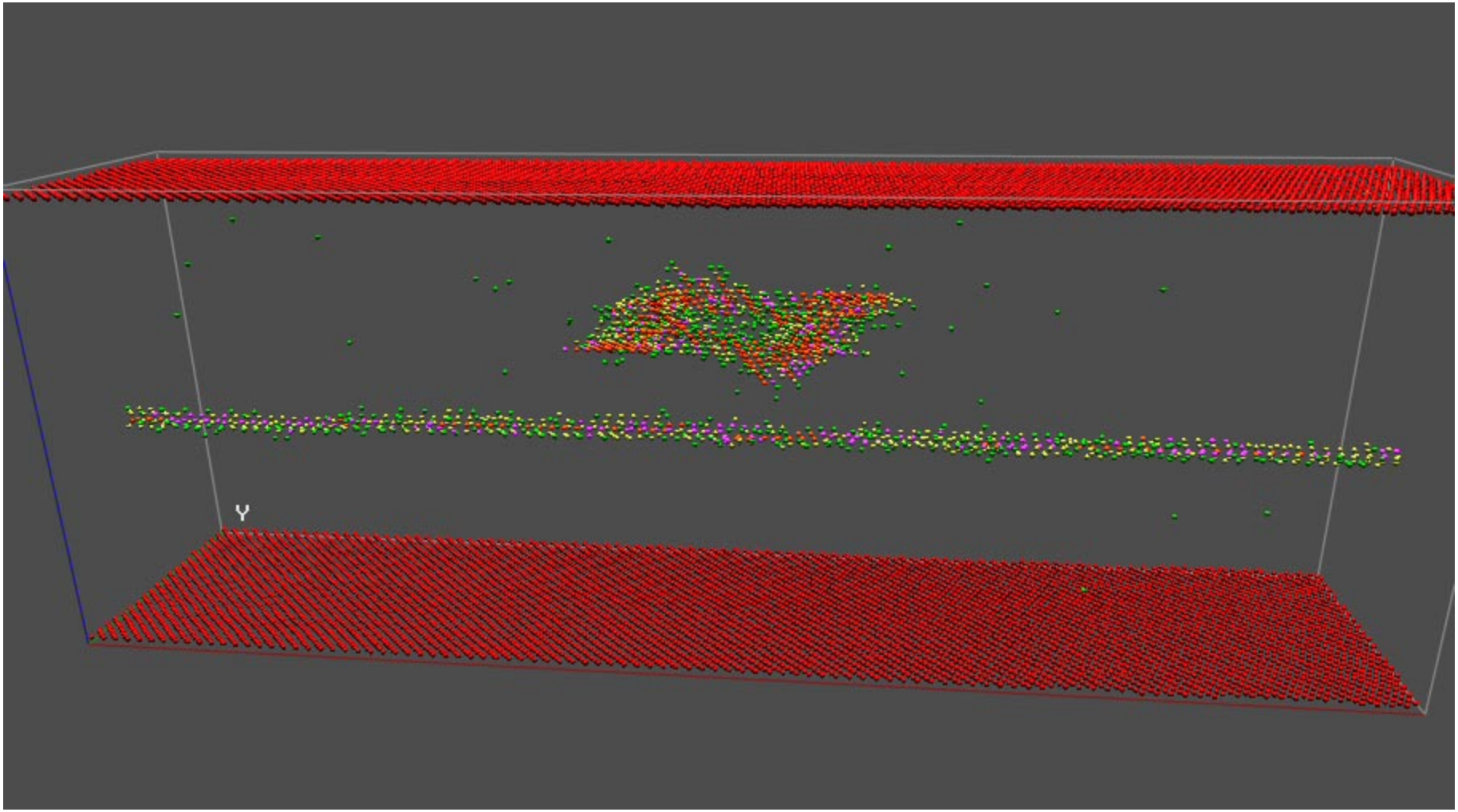
- void acts as strong shearable obstacle
- Bypass: dislocation annihilation & re-nucleation, creating a surface ledge

Screw dislocation motion in α-Fe: 400 MPa



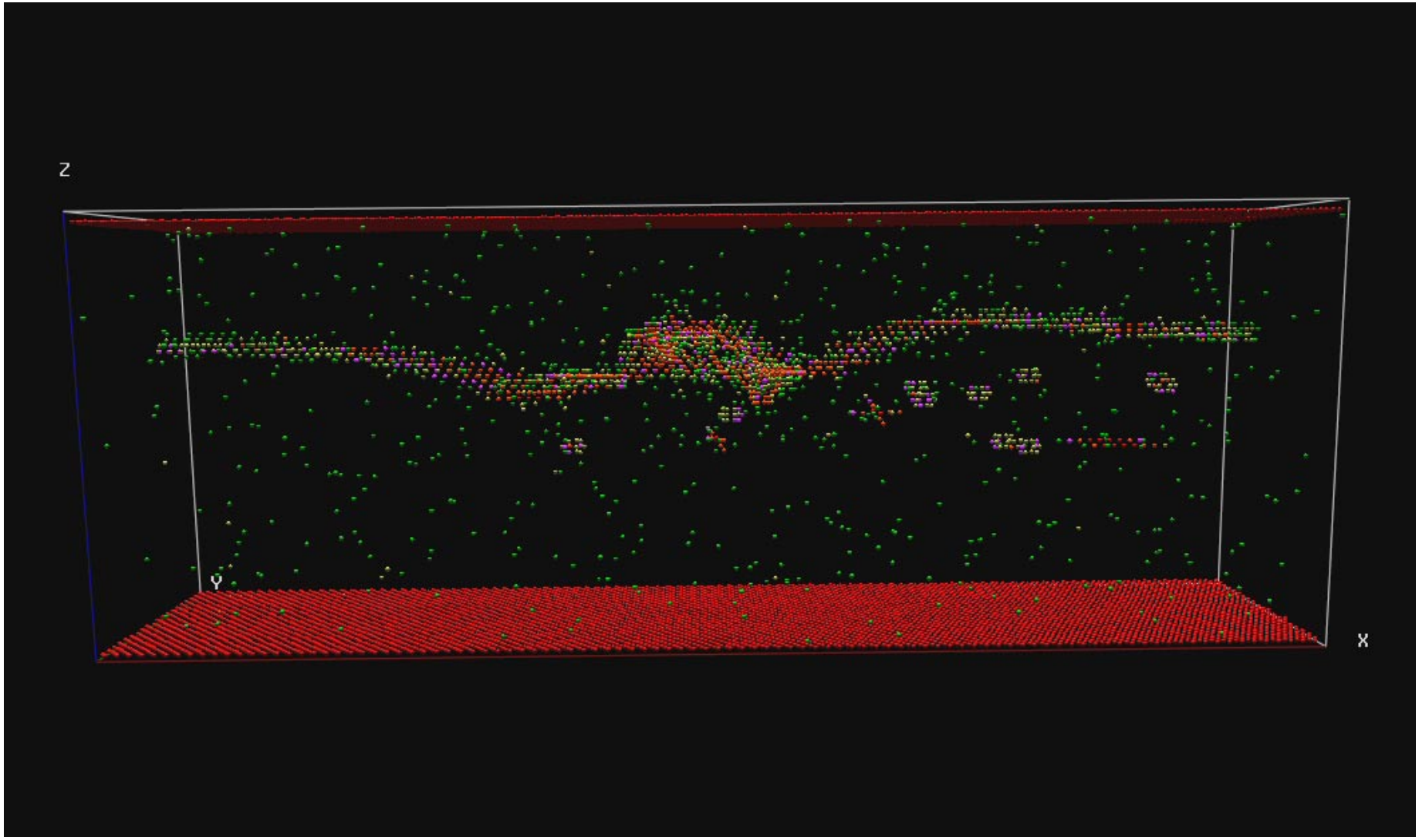
- Screw dislocation moves by double kink nucleation (as expected), glide along <112> direction, with frequent cross-slip - and debris field left behind

Screw dislocation interaction with $\langle 100 \rangle$ loop in α-Fe: 750 MPa



$\langle 100 \rangle$ loop is sheared into two $\frac{1}{2}\langle 111 \rangle$ loops, one is absorbed forming a spiral, the other one pins the dislocation

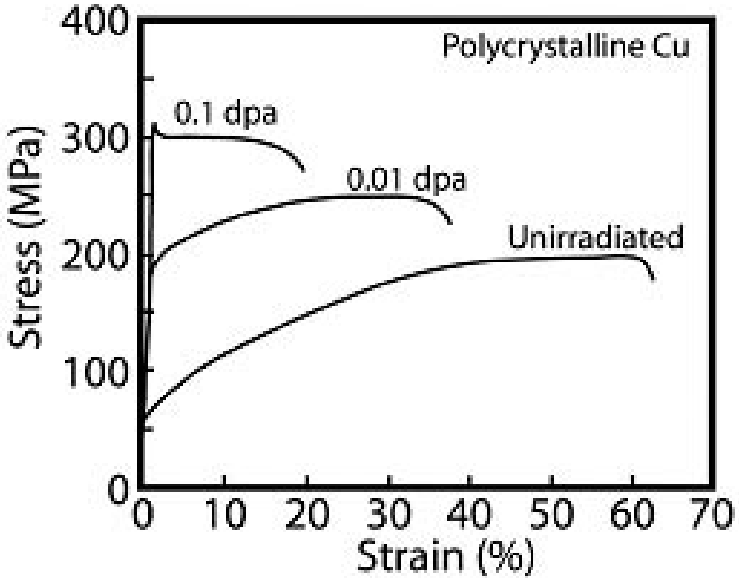
Screw dislocation interaction with ⟨100⟩ loop in α-Fe: 1000 MPa



Screw dislocation bypasses loop at higher applied stress and cross-slips to free surface - ⟨100⟩ loop remains

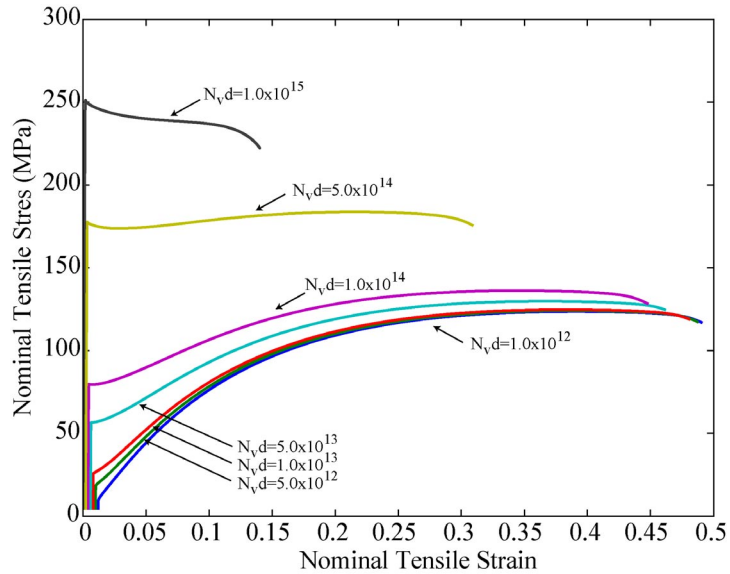
Isotropic polycrystal plasticity model for irradiated metals

Tension Experiments



B. N. Singh et al,
J. Nucl. Mat. **224,** 131 (1995).

Tension Simulations



- Isotropic polycrystal plasticity incorporates coarse grained scaling laws governing dislocation density evolution and interactions determined for single crystals
- Dislocation - (radiation damage) defect interactions can be included, based on MD simulations and/or experimental values
- Resulting models can be further modified to include the effects of dispersed particles, solute atoms, and other known resistance mechanisms

Constitutive modeling framework - irradiated steels

- **Large deformation crystal plasticity model developed for modeling the stress-strain behavior of irradiated steels**

- The model calculates the effective plastic strain rate via Orowan's eq:

$$\frac{d\vec{\varepsilon}_p}{dt} = \rho_d b \vec{v}_d$$

ρ_d - dislocation density,
b - Burgers vector
V_d - average dislocation velocity

-The dislocation density evolves by:

$$\frac{d\rho_d}{dt} = \left(\frac{2}{bd_d} - \rho_d \frac{R_c}{2b}\right)\frac{d\vec{\varepsilon}_p}{dt}$$

d_d - dislocation loop size
R_c - capture radius

- The dislocation velocity is given by:

$$\vec{v}_d = v_o\left(\frac{\vec{\sigma}}{\mu b\sqrt{\alpha\rho_d + \beta N_v d}}\right)^{1/m}$$

N_v - radiation defect cluster number density
d - radiation defect cluster size
β - strengthening coefficient

Modeling Framework Continued

Dislocation loop size evolution

$$\dot{d}_d = d_d \frac{\dot{\rho}_d}{\rho_d} - \delta d_d^3 \dot{\rho}_d$$

δ - source multiplication constant

Evolution of defect density by dislocation cutting

$$\frac{d(N_v d)}{dt} = \left(\frac{b}{d}\right) N_v d^2 \rho_d \vec{v} = (N_v d) \frac{d\vec{\varepsilon}^p}{dt}$$

Conservation of defect density

$$N_v d^3 = N_v(_{t=0}) d^3(_{t=0})$$

Strength of defects as a function of size

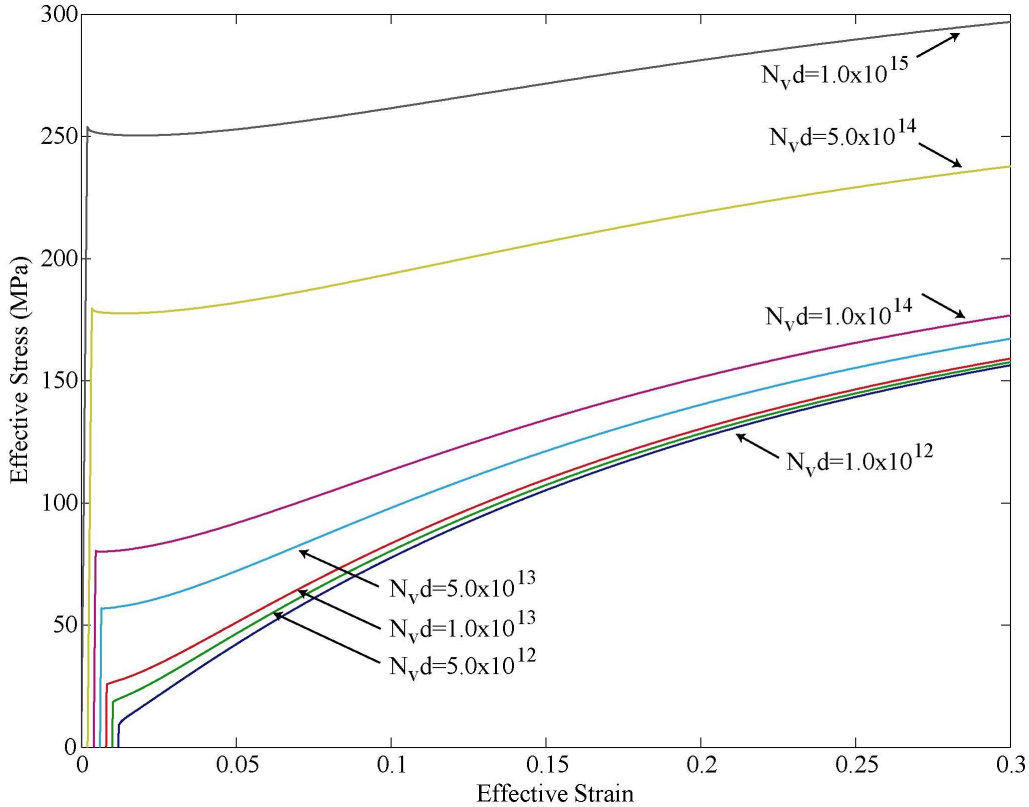
$$\beta = 1 - \exp\left[-\left(\frac{d}{d_{ref}}\right)^n\right]$$

d_{ref} - reference defect size

n - defect size sensitivity

Constitutive model - irradiated steels

Single Material-Point Calculation



- **Model reproduces experimental observations of increasing yield stress, appearance of a yield point and decreased work-hardening**

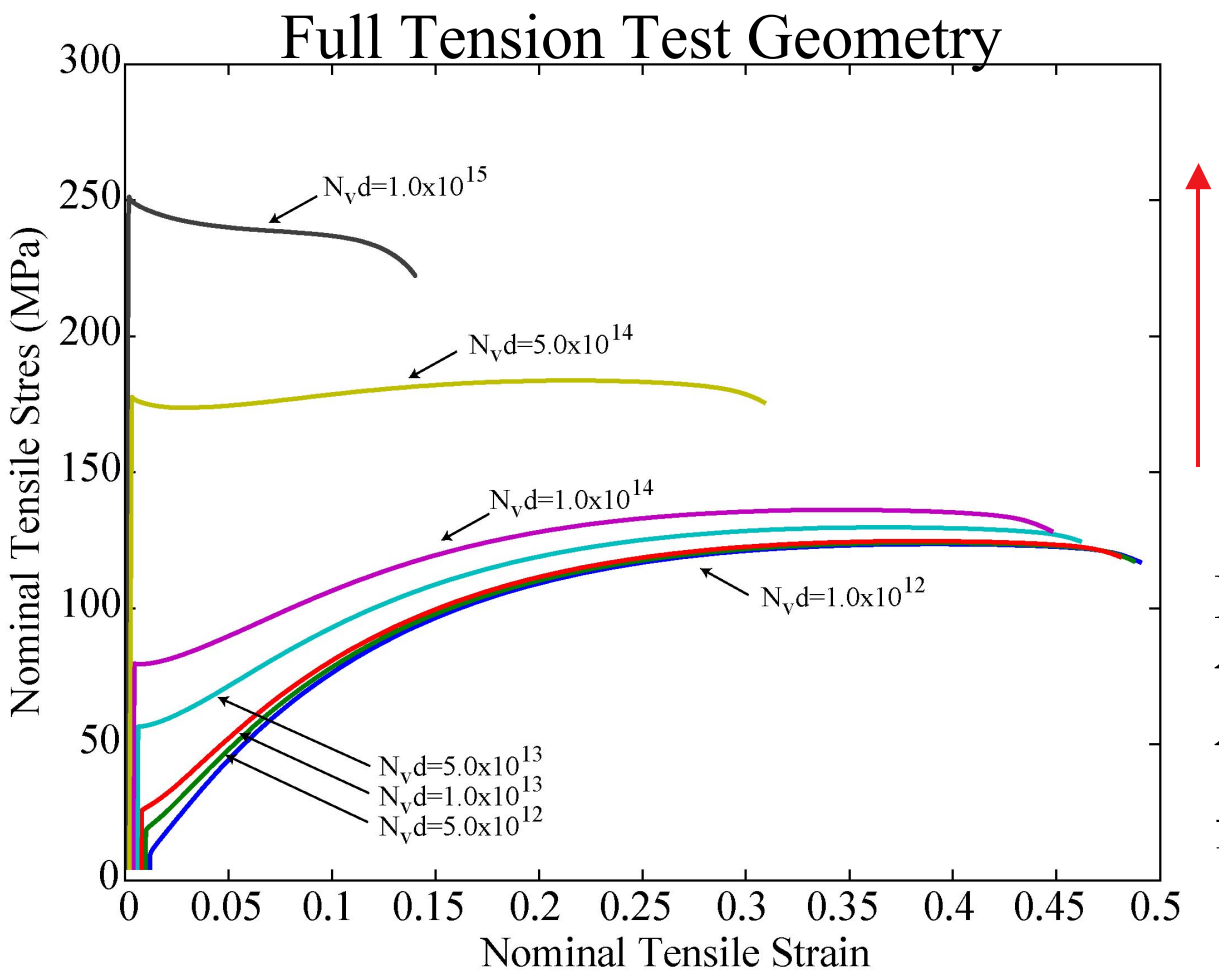
Increasing defect cluster density

Hardening-Softening Characteristics

$$\frac{d\vec{\sigma}}{d\vec{\varepsilon}^{p}} = \left[\left(\frac{\alpha}{2(\alpha\rho_d + \beta N_v d)} - \frac{m}{\rho_d}\right)\left(\frac{2}{bd_d} - \rho_d \frac{R_c}{2b}\right) + \frac{N_v d}{2(\alpha\rho_d + \beta N_v d)}\left(\beta + \frac{n}{2}(1-\beta)\ln(1-\beta)\right)\right]\vec{\sigma}$$

Preliminary constitutive model - irradiated steels

- **Constitutive model in FEM, full tension test geometry simulation reproduces experimental observations of increasing yield stress, appearance of a yield point and decreased work-hardening**



Increasing defect cluster density

Plastic instability in tension geometry leads to flow localization and failure

Summary

- **Dispersed barrier and cascade induced source hardening models generally used to describe radiation hardening ($\Delta\sigma_y$) and yield drops - significant questions remain - DBH model not applicable to post-yield flow behavior, a' values not always consistent**

- **MD simulations can provide improved understanding of dislocation - obstacle interactions, fates and α' (Note, MD probes very high strain rate interactions & can not model climb, diffusion mediated bypass)**

- **Introduced an isotropic, polycrystal plasticity based framework for the constitutive response of irradiated metals - incorporation into FEM generally reproduces measured tensile data**

A look ahead

- **Characterize screw dislocation - obstacle interaction (both bcc and fcc metals), including ODS particles (improve understanding of creep resistance)**

- **Kinetic Monte Carlo and/or Dislocation Dynamics modeling of thermal bypass mechanisms (vacancy diffusion, cross-slip) associated with slow strain rate and creep related processes**

- **Additional experimental work (including in-situ TEM deformation studies) to completely characterize pre- and post-deformation microstructure and constitutive properties**

- **Account for multiple defect interactions in polycrystal plasticity based constitutive model**