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Title: Dislocation Dynamics Model of the Plastic Flow of fcc Polycrystals from Quasi-static to High Strain Rates

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ABSTRACT

A new internal state variable model of plastic flow is discussed. The state variables are the mobile and immobile (network) dislocation densities. The model is comprised of three coupled ordinary differential equations: a kinetic equation, which relates the strain rate to the stress, the state variables, the temperature, and the density, and two dislocation evolution equations. The evolution equations account for dislocation generation, storage of dislocations in the network and on grain boundaries, and several dynamic recovery processes. The kinetic equation is not a Van't Hoff-Arrhenius thermal activation model, as is the case for all other rate-dependent strength models, but rather a mean first-passage time model that extends the validity of the kinetic equation to arbitrarily high strain rates. The dislocation recovery processes in the model include mobile-immobile and mobile-mobile annihilation, and single cross-slip plus screw-screw annihilation. Dislocation are generated in the model by Frank-Read sources, the Koehler mechanism (double cross-slip followed by loop/dipole formation), and grain boundary nucleation. Preliminary results on copper deformation are presented.

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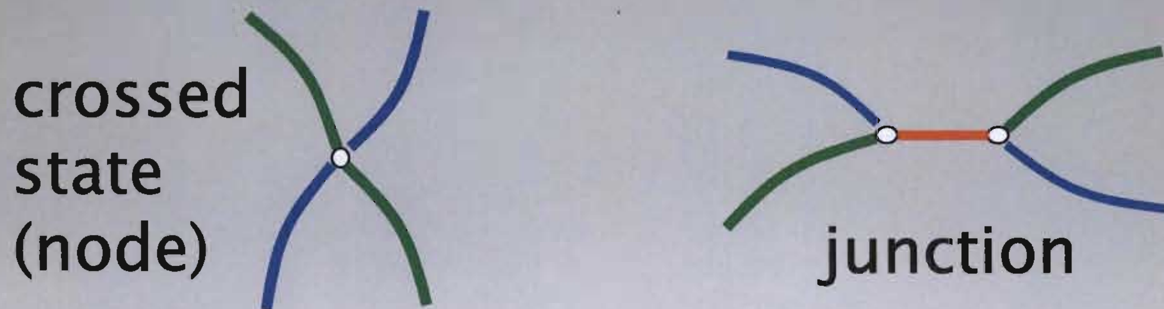
Computational Physics
LANL

Model overview

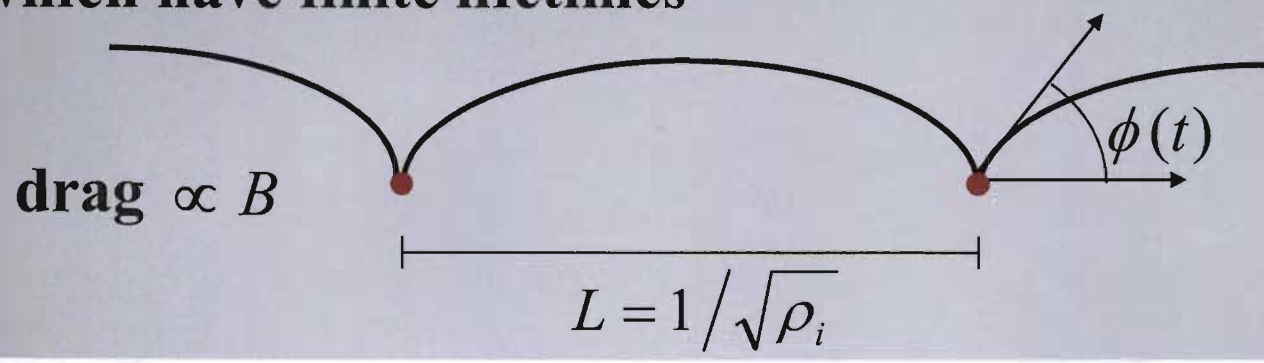
- **Currently applicable to pure fcc polycrystalline metals**
- **Two internal state variables**
  ρ_m – **mobile dislocation density**
  ρ_i – **immobile density**
- **Comprised of 3 coupled ODEs**
  1. **Kinetic equation** $\dot{\varepsilon}(\sigma, \rho_m, \rho_i, T, P)$
  2. **Mobile and immobile dislocation evolution equations**
     $\dot{\rho}_{m,i} = g_{m,i}(\sigma, \dot{\varepsilon}, \rho_m, \rho_i, T, P)$
     Account for: dislocation generation
     network & grain boundary storage
     dynamic recovery

Kinetic equation

Rate controlling mechanism is the intersection of attractive, non-coplanar mobile & immobile dislocations



Applied stress bows dislocations between nodes/junctions which have finite lifetimes



High strain rates require MFPT theory

It is generally accepted that the intersection controlled strain rate is related to the stress according to

$$\dot{\varepsilon} = \dot{\varepsilon}_0 \exp\left\{-\frac{E(\sigma)}{kT}\right\}$$

Van't Hoff-Arrhenius thermal activation (VATA)

but VATA is only valid for $\dfrac{E(\sigma)}{kT} >> 1$

High $\dot{\varepsilon}$ $\Rightarrow$ **large** σ $\Rightarrow$ $\dfrac{E(\sigma)}{kT} << 1$

VATA→ mean first-passage time (MFPT) model of dislocation intersection

$\exists$ local stress fluctuations at nodes/junctions. Distribution & correlation time needed for MFPT calculation.

- $T = 0$ node/junction dissolution condition $\sigma \geq \sigma_c$

- $T > 0$ local stress fluctuation $+ \sigma \geq \sigma_c$ **Fluctuation distribution** is approximated as Gaussian

$$\left\langle \sigma_{local}^2 \right\rangle^{1/2} \sim \sqrt{G k T / b^3} \sim$$ rms atomic displacement

Fluctuation correlation time is $\bar{\nu}^{-1}$ $\bar{\nu} =$ avg phonon frequency

MFPT (σ fluctuations) → Kinetic Equation

MFPT calculation *specific* to dislocation intersection → $t_w = \bar{\nu}^{-1} \dfrac{\mathcal{P}}{\ln^2(1-\mathcal{P})}$ **mean node/junction lifetime**

$$\mathcal{P}(\sigma, \rho_i, T, P) = \frac{1}{2} erfc\left\{ \frac{\kappa b L}{\sqrt{G b k T}} (\sigma_c - \sigma) \right\} \qquad L = 1/\sqrt{\rho_i}$$

$$\sigma_c = \frac{5}{8\pi} \phi_c G \frac{b}{L} \ln\left(\frac{L}{b}\right) \qquad \phi_c \approx 1/2 \approx 30^\circ \text{ Cu}$$

Kinetic equation $$\dot{\varepsilon} = \dot{\varepsilon}_0 \left\{ \frac{\ln^2[1-\mathcal{P}(\sigma)]}{\mathcal{P}(\sigma)} - \frac{\ln^2[1-\mathcal{P}(-\sigma)]}{\mathcal{P}(-\sigma)} \right\}, \quad \dot{\varepsilon}_0 = b \rho_m L \bar{\nu}$$

Kinetic equation - limits

- $\dfrac{E(\hat{\sigma}_c - \hat{\sigma})^2}{kT} >> 1 \qquad E = \kappa^2 G b L^2 \qquad \hat{\sigma} = \sigma / G$

$$\dot{\varepsilon} = \dot{\varepsilon}_0 \frac{G}{2\sigma_c}\left(\frac{kT}{\pi E}\right)^{1/2} \exp\left\{-\frac{E(\hat{\sigma}_c - \hat{\sigma})^2}{kT}\right\}$$

Van't Hoff-Arrhenius exponential with $\sqrt{T}$ pre-factor

- $\sigma >> \sigma_c \qquad \dot{\varepsilon} = \dot{\varepsilon}_0 \left(\dfrac{E}{kT}\right)^2 \hat{\sigma}^4$

For $\dot{\varepsilon} = const \qquad \sigma \sim T^{1/2} \Rightarrow$ **thermal hardening**

Dislocation Evolution Equations

$$\dot{\rho}_{m,i} = g_{m,i}(\sigma, \dot{\varepsilon}, \rho_m, \rho_i, T, P)$$

Storage & Recovery

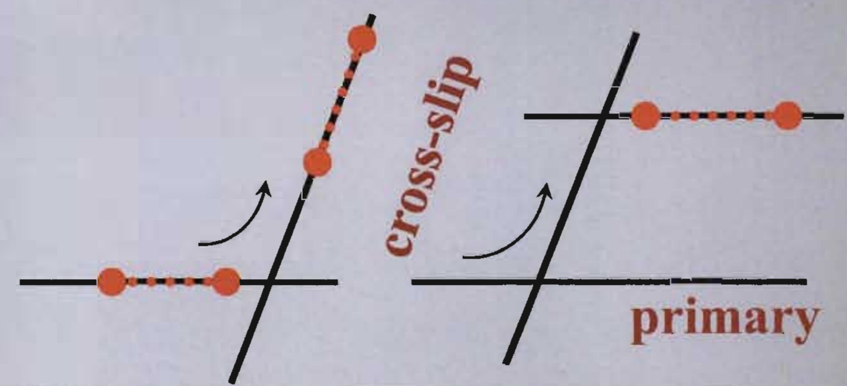
NETWORK STORAGE = JUNCTION FORMATION

MOBILE--MOBILE ANNIHILATION

GRAIN BOUNDARY STORAGE

MOBILE--IMMOBILE ANNIHILATION

CROSS-SLIP + SCREW--SCREW ANNIHILATION

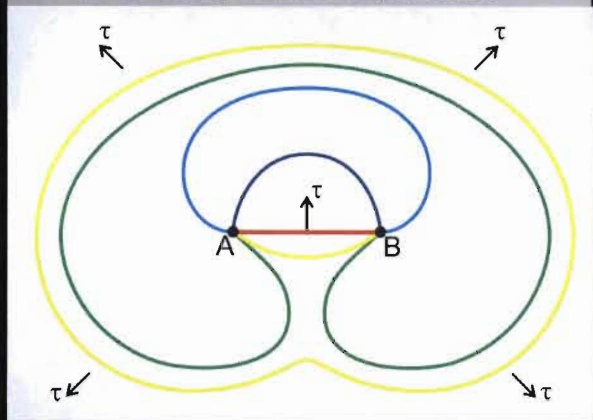


Dislocation Evolution Equations

$$\dot{\rho}_{m,i} = g_{m,i}(\sigma, \dot{\varepsilon}, \rho_m, \rho_i, T, P)$$

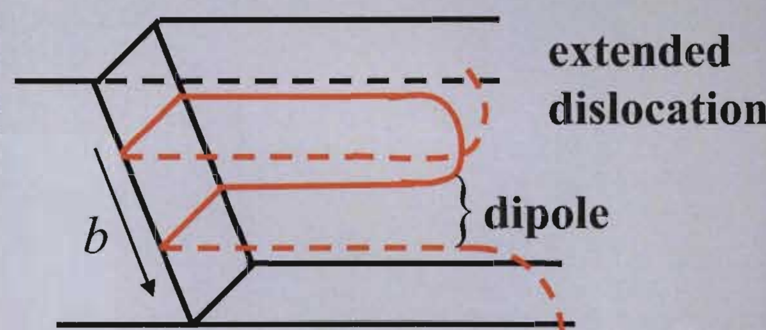
Generation

FRANK-READ



KOEHLER MECHANISM DOUBLE CROSS-SLIP + LOOP GENERATION

DOUBLE CROSS-SLIP + DIPOLE FORMATION



GRAIN BOUNDARY NUCLEATION

Network Evolution

$$\frac{d\rho_i}{dt} = g_{s\partial}\frac{\dot{\varepsilon}}{bD} + (g_{sn} - g_{ami})\frac{1}{b}\sqrt{\rho_i}\,\dot{\varepsilon}$$

$$+ g_{FR}\frac{D}{b\,d_{FR}}\,\dot{\varepsilon}\,\frac{d}{dt}\int_0^{(t-\tau)\theta(t-\tau)}\sqrt{\rho_i(t')}\,dt'$$

$$- g_{ax}\frac{h_c}{b}\rho_i\,\dot{\varepsilon} - g_{tx}\,\rho_m\,\bar{\nu}\exp\{-E_x(\sigma)/kT\}$$

$$+ g_{xx}\frac{D}{d_{xx}}\exp\{-E_{xx}(\sigma,2)/kT\}\,\bar{\nu}\,\frac{d}{dt}\int_0^{t-\tau}\rho_m(t')\,dt'$$

$$+ \frac{2}{\pi}g_{xx}\frac{1}{b\,d_{xx}}\exp\{-E_{xx}(\sigma,1)/kT\}\,\bar{\nu}\,\dot{\varepsilon}$$

$$\times\frac{d}{dt}\left\{t^2\,\theta(\tau-t) + \tau(t-\tau/2)\,\theta(t-\tau)\right\}$$

$D =$ **grain diameter**

$$\tau = \frac{bD\rho_m}{2\dot{\varepsilon}}$$

$E_x, E_{xx} =$ **activation energies**

Mobile Dislocation Evolution

$$\frac{d\rho_m}{dt} = -g_{amm}\frac{1}{b}\sqrt{\rho_m}\,\dot{\varepsilon} - g_{s\partial}\frac{\dot{\varepsilon}}{bD} - (g_{sn} + g_{ami})\frac{1}{b}\sqrt{\rho_i}\,\dot{\varepsilon}$$

$$+ g_{FR}\frac{D}{b\,d_{FR}\,\tau^2}\,\dot{\varepsilon}\,\frac{d}{dt}\int_{(t-\tau)\theta(t-\tau)}^{t}(t-t')^2\sqrt{\rho_i(t')}\,dt'$$

$$-g_{ax}\frac{h_c}{b}\rho_i\,\dot{\varepsilon} - g_{tx}\,\rho_m\,\bar{\nu}\exp\left\{-E_x(\sigma)/kT\right\}$$

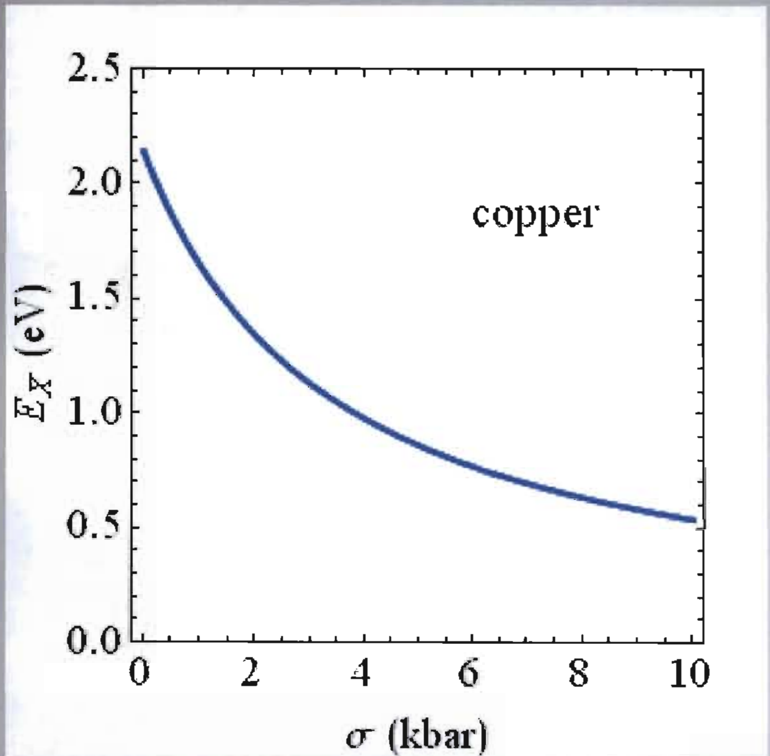
$$+ g_{xx}\frac{1}{2b\,d_{xx}}\exp\left\{-E_{xx}(\sigma,2)/kT\right\}\bar{\nu}\,\dot{\varepsilon}\,\frac{d}{dt}\left\{t^2\theta(\tau-t)+\tau^2\theta(t-\tau)\right\}$$

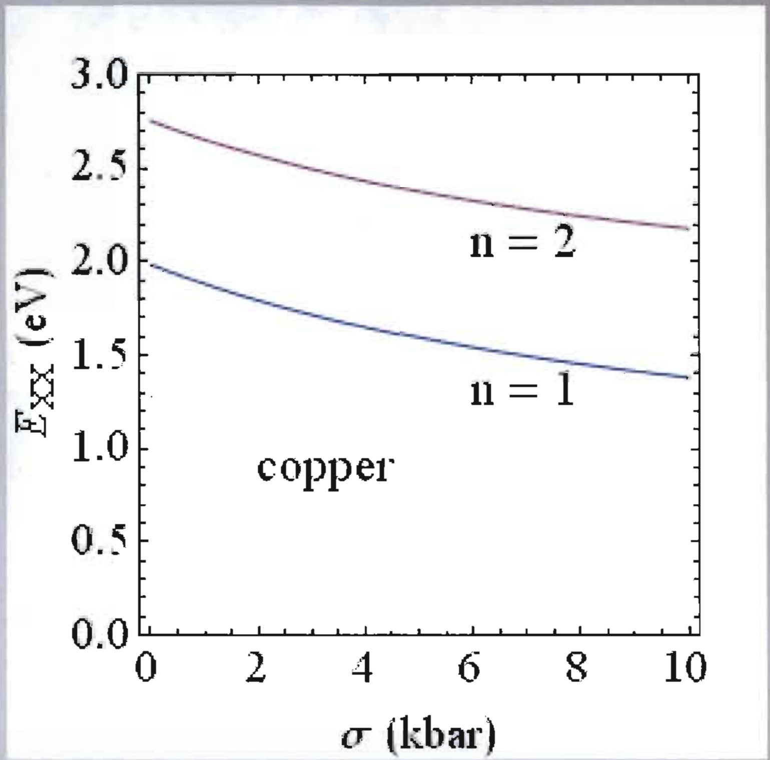
cross-slip terms

$$\frac{d\rho_{m,i}^{x,xx}}{d\varepsilon} \sim \frac{\bar{\nu}}{\dot{\varepsilon}}\exp\left\{-\frac{E_{x,xx}}{kT}\right\}$$

cross-slip enhanced at high T & low rates

Single & double cross-slip activation energies

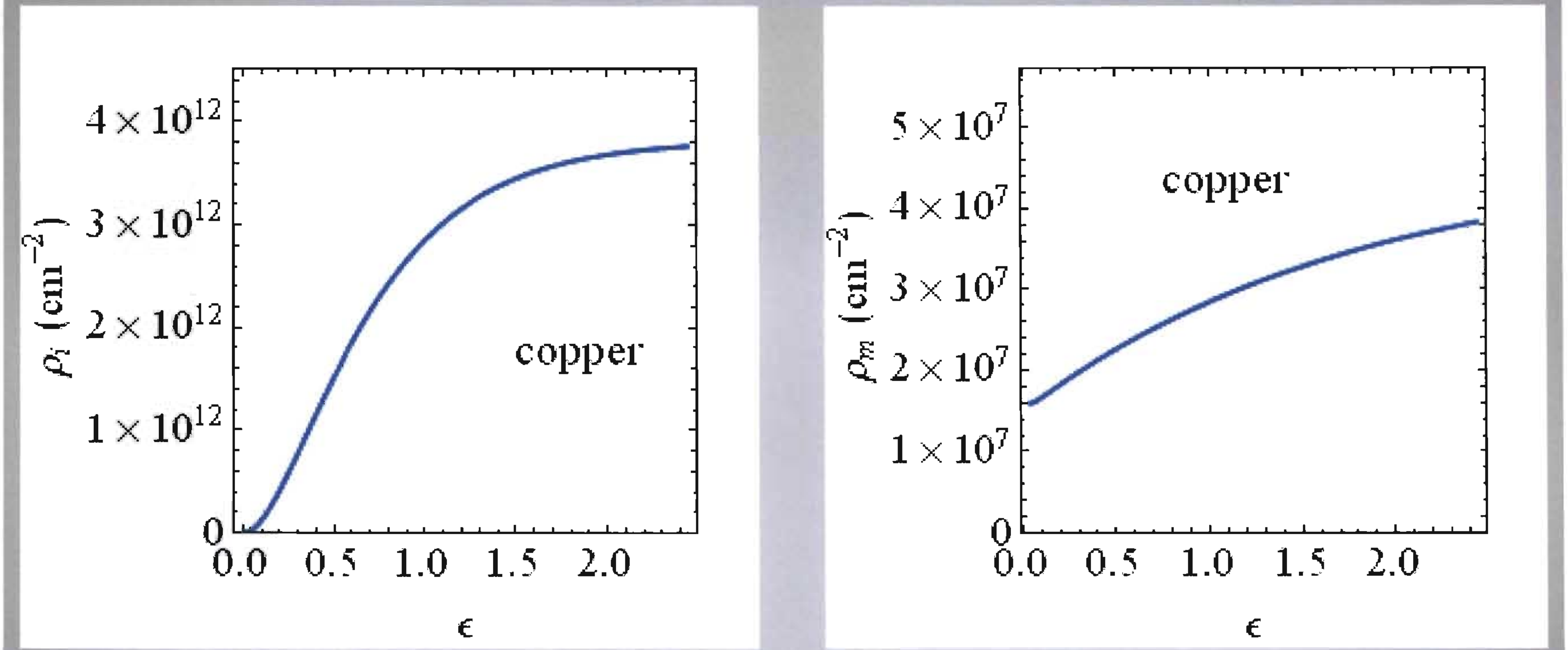




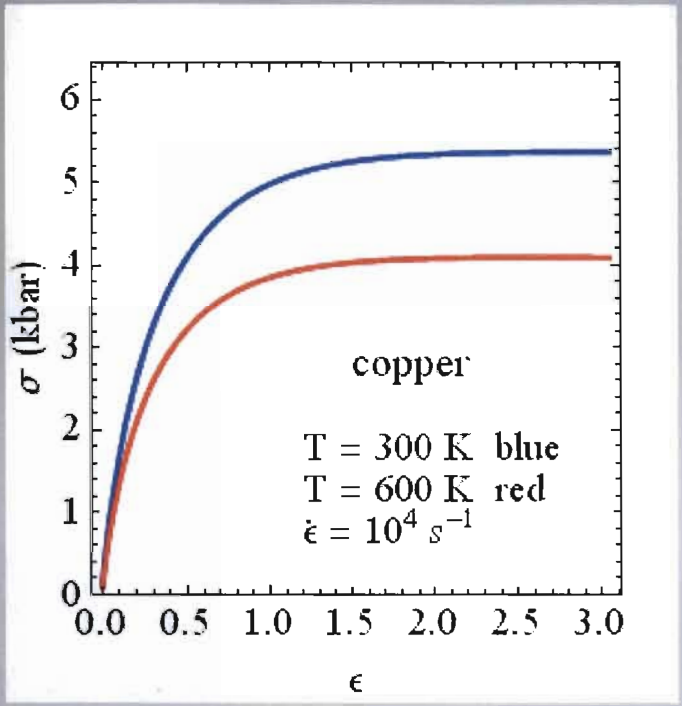
Single cross-slip:
modified Friedel-Escaig

Double cross-slip:
extended Friedel-Escaig

Preliminary results on Cu
Low T: cross-slip not exercised

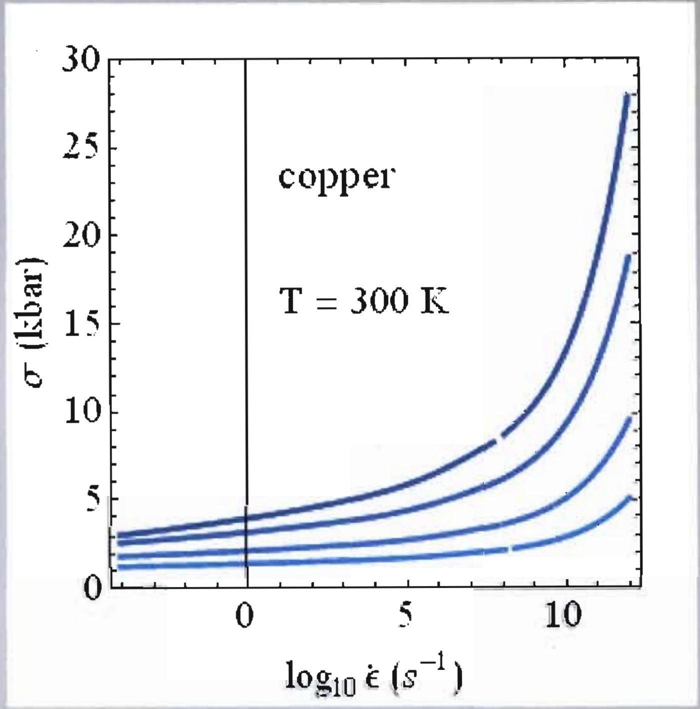


Preliminary results on copper



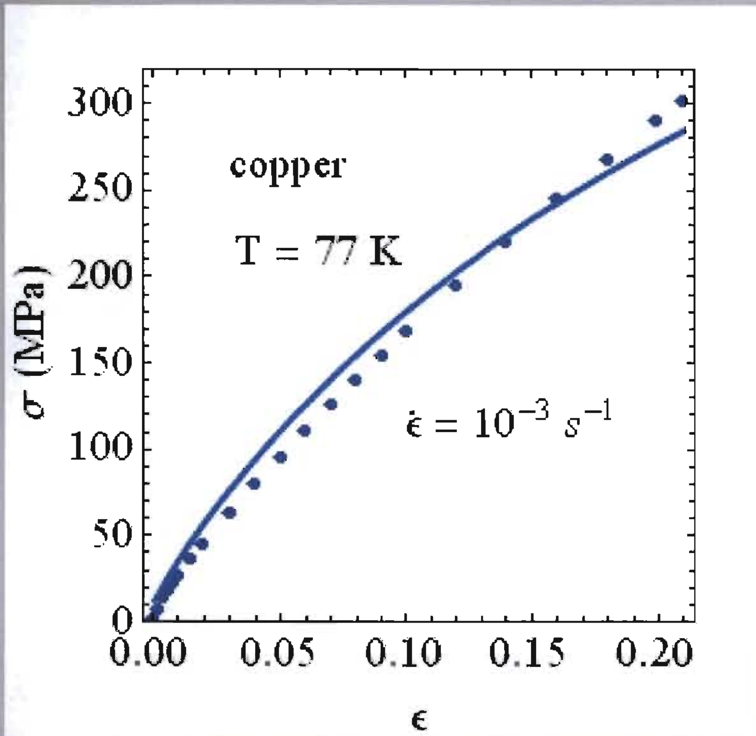
Thermal softening is due to T-dependence of mobile-immobile interactions

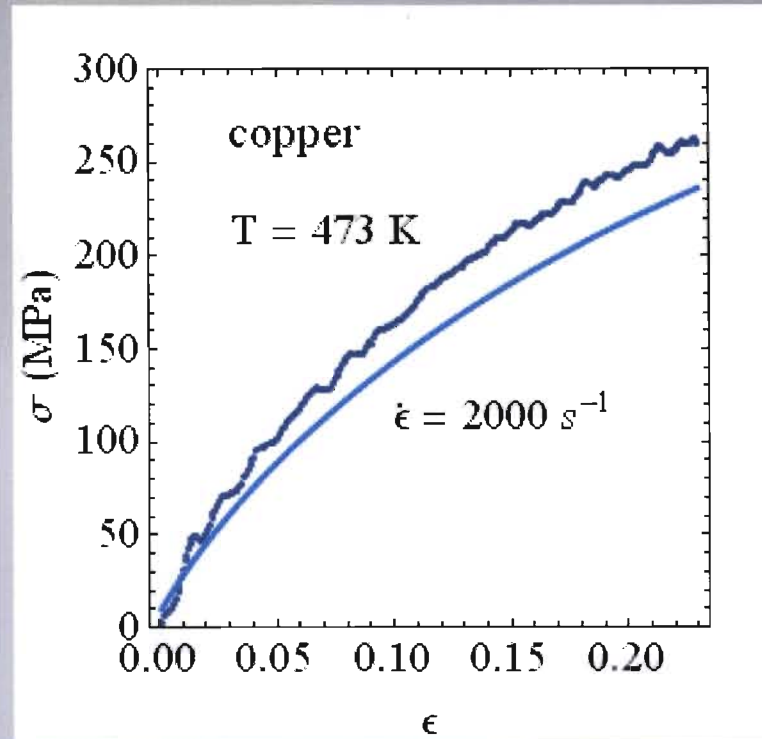
Flow stress vs rate for strains $0.1,\ 0.2,\ 0.5,\ \varepsilon >> 1$



Increase in rate sensitivity not due to dislocation drag

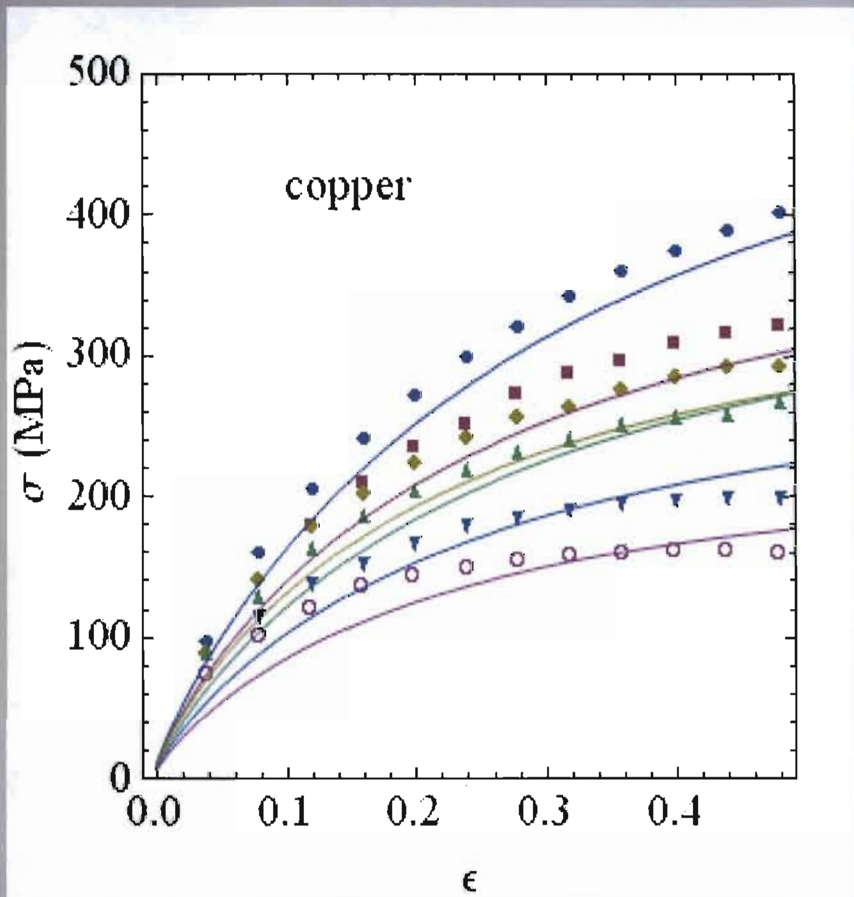
Stress-strain: model vs data on OFE copper





Did not optimize parameter values

Comparison with PTW model



solid circles: $298\,K,\ 2000\ s^{-1}$

squares: $298\,K,\ 0.1\ s^{-1}$

diamonds: $298\,K,\ 0.001\ s^{-1}$

up triangles: $673\,K,\ 2000\ s^{-1}$

down triangles: $873\,K,\ 2000\ s^{-1}$

open circles: $1073\,K,\ 2000\ s^{-1}$

Future Directions

- Cu model: turn on cross-slip
- Include dislocation drag ➢ phonon drag, flutter, …
- Account for dependence of strength on material density
  - ➢ Investigate shear modulus scaling
    $\sigma(\ldots,\rho)\,/\,G(\rho,T)$ is assumed independent of density
- Compute fraction of plastic work dissipated (usually taken to be 100%)
- Calculate dislocation cell formation due to mesoscale stress fluctuations
- May be necessary to "model the model"