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A Dislocation Dynamics Model of the Plastic Flow of fcc Polycrystals: Dislocation Intersection Processes

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Plastic Flow Models

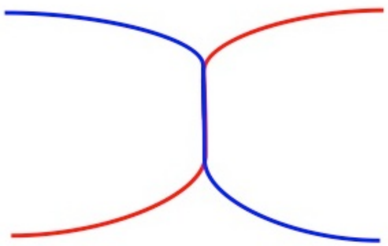
- Difficulty accounting for material strength behavior at high strain rates, temperatures, and pressures
  - Of interest for shock loading
  - Plastic strain rates of 10^6 s^{-1} and above
  - Pressures from ambient to 1000GPa
  - Temperatures from zero to melt
- Van't Hoff-Arrhenius Equation

$$\Gamma^{-1} = f_a \exp\left(-\frac{E}{k_B T}\right)$$

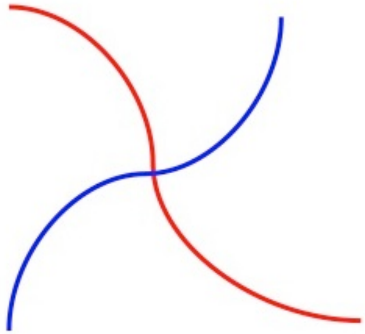
  - Determine the lifetime of a dislocation node
    - The decay rate of a metastable state with respect to thermal fluctuations.
  - Only valid when the height of the potential barrier is large in comparison to the thermal energy: $E/k_B T >> 1$
    - As stress increases the potential barrier must decrease so that the plastic strain rate can increase.

Plastic Flow Models

- Difficulty accounting for specific mesoscale deformation behavior
  - Mesocale phenomena determine macro-scale material behavior
  - Dislocation generation and annihilation
  - Frank-Read sources
  - Cross-slip



- Mobile-immobile dislocation pairwise intersection
  - Primary cause of work-hardening in fcc metals
  - Predominant rate-controlling mechanism in fcc metals
  - Junctions
  - Crossed state (node)
    - Crossed states form much more frequently than junctions



J. Friedel, 1964; Bulatov, 2006; Wickham, 1999

Model Overview

- Two internal state variables
  - Mobile dislocation density: ρ_m
  - Immobile dislocation density: ρ_i

$$\rho_{tot} = \rho_i + \rho_m$$

- 3 coupled ODEs
  - Mobile and immobile dislocation evolution equations
  - Kinetic equation
    - Relates stress and plastic strain rate
    - Describes the dissociation of mobile-immobile dislocation intersections
    - Based on a mean first passage time (MFPT) framework

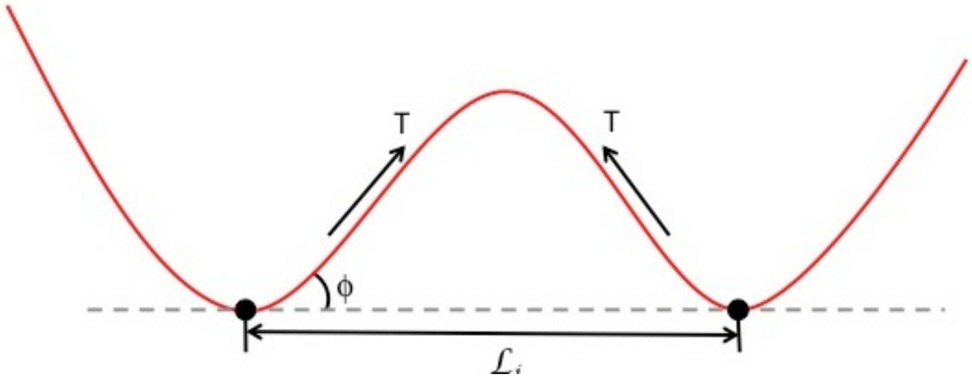
Applied Stress

- Effective applied stress: $\hat{\sigma} = \sigma - \sigma_b$
- Back stress: $\sigma_b = g_b b G(\rho, T)\sqrt{\rho_i}$
- Critical applied shear stress
  - Stress required to dissociate nodes and remobilize stalled mobile dislocations at zero temperature.

$$\mathcal{F}_c = 2\mathcal{T}\phi_c = \sigma_c b \mathcal{L}_i$$

$$\mathcal{T} = \frac{5}{16\pi} G b^2 \ln\left(\frac{\mathcal{L}_i}{b}\right)$$

$$\sigma_c = \frac{5}{8\pi}\phi_c G b \sqrt{\rho_i} \ln\left(\frac{1}{b\sqrt{\rho_i}}\right)$$



$$\mathcal{L}_i = \frac{1}{\sqrt{\rho_i}}$$

Hirth and Lothe, 1968; Burgers *et al.*, 1935; Seeger, 1955

Mean First Passage Time (MFPT) Theory

- Breakdown of standard activation theory $\dot{\epsilon} = \dot{\epsilon}_o \left\{ -\frac{E(\sigma)}{kT} \right\}$
  - Only valid for: $\frac{E(\sigma)}{kT} >> 1$
  - At high strain rates, stress increases and: $\frac{E(\sigma)}{kT} << 1$
- MFPT is the average time required for a stochastic process, *f(t)*, with or without memory, to first leave a prescribed open domain.
  - Process can be described by the conditional probability: $P_\Omega(f, t|f_0)$

$$t_\Omega(f_0) = \int_0^\infty \int_\Omega P_\Omega(f, t|f_0) df\, dt.$$

  - Stochastic process = thermally-driven force component
  - Average time = time to remobilize the mobile dislocation
    - Mean node lifetime
  - Domain = open time-dependent interval that ends when a critical force fluctuation is achieved and the node dissociates.

Thermally-Driven Force Fluctuations

- At finite temperature, the total force between two intersecting dislocations: $\mathcal{F}(\sigma, \sigma_b, t) + f(t) \geq \mathcal{F}_c$
  - Applied forces plus thermal vibrations
  - Must be greater than or equal to a critical force to dissociate the node.
- Consider localized vibrational modes
  - An intersection node is an extended defect within the crystal
    - Localized mode frequencies are shifted above the frequency band of a perfect crystal
    - Amplitudes die out rapidly with increasing distance from the defect
    - Motions of defects and nearest neighbors are well-approximated with only localized modes.
    - Distribution of force fluctuations between dislocations is nearly Gaussian

$$\langle f^2 \rangle = \frac{1}{2} G b k_B T \sum_{i=1}^{n} \alpha_i^2 \equiv G b k_B T / \kappa \quad \mathcal{P}(f) \approx \frac{1}{\sqrt{2\,\pi\,\langle f^2 \rangle}} \exp\left\{ -\frac{f^2}{2\,\langle f^2 \rangle} \right\}$$

Mean Remobilization Time

- Product of the probability of node formation, and mean node lifetime.

$$t_r = \underbrace{\frac{1}{2}\left(1 + erf\sqrt{\frac{\mathcal{E}}{k_B T}}\right)}_{\text{Probability of node formation at } t=0;\ f(0) < f_c(0)} \underbrace{\int_0^\infty \exp\left\{-\frac{1}{\tau}\int_0^t \mathcal{D}_\tau(t')\,dt'\right\} dt}_{\text{Mean node lifetime}}$$

Probability of node formation at t = 0; f(0) < $f_c(0)$

Mean node lifetime

$$\mathcal{D}_\tau(t) = \int_{f_c(t)}^\infty \mathcal{P}(f)\,df \qquad \int_0^\infty t\,\mathcal{D}(t)dt = \int_0^\infty t\mathcal{S}(t)\,\mathcal{D}_\tau(t)\,\frac{dt}{\tau}$$

$$\mathcal{D}_\tau(t) = \frac{1}{2}\left\{1 - erf\left[\sqrt{\frac{\mathcal{E}}{k_B T}}\left(1 - \frac{\hat{\sigma}}{\sigma_c}\left(1 - e^{-t/t_B}\right)\right)\right]\right\} \qquad \mathcal{S}_t(t) = \exp\left\{-\frac{1}{\tau}\int_0^t \mathcal{D}_\tau(t')\,dt'\right\}$$

- Instantaneous Bow-out: B = 0
  - Critical force fluctuations are no longer time dependent

$$t_r = \frac{1 - \mathcal{D}_\tau(0)}{\mathcal{D}_\tau(\hat{\sigma})}\tau$$

High and Low Stress Limits

- Low stress limit: $\hat{\sigma}/\sigma_c << 1$
  - Recover the Arrhenius exponential – valid at low stresses

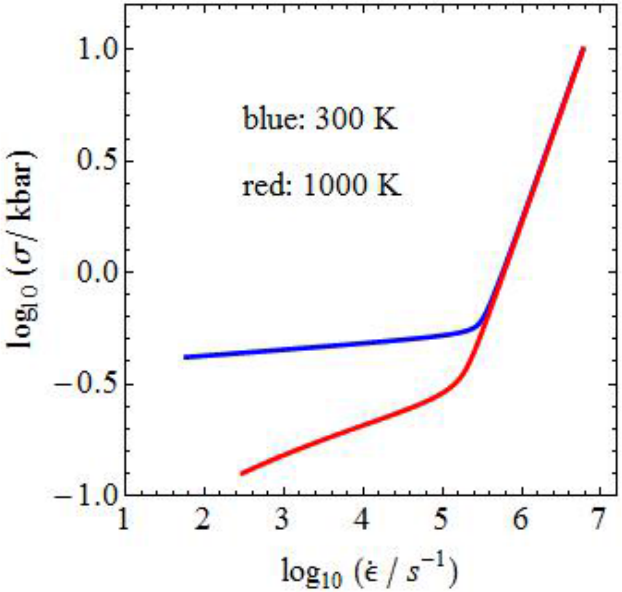
$$t_r^{-1} = \frac{1}{2\tau}\left(\frac{k_B T}{\pi \mathcal{E}}\right)^{\frac{1}{2}} \exp\left\{-\frac{\mathcal{E}}{k_B T}\left(1 - 2\frac{\hat{\sigma}}{\sigma_c}\right)\right\}$$

- High stress limit: $\hat{\sigma}/\sigma_c >> 1$

$$\frac{t_r}{\tau} = \frac{t_B}{\tau}\frac{\sigma_c}{\hat{\sigma}} + 1$$

Kinetic Equation

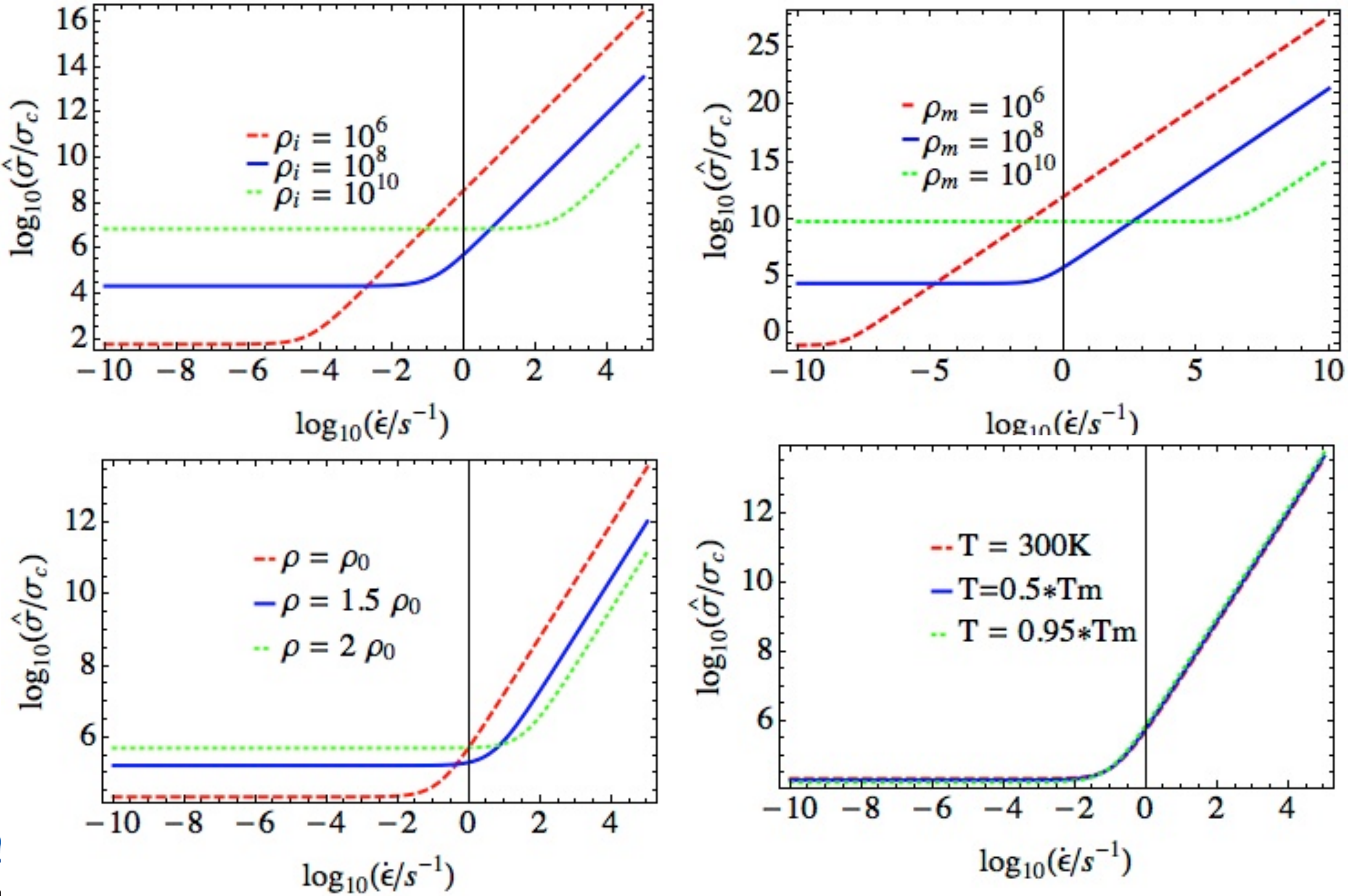
$$\dot{\epsilon} = \frac{\zeta\, b\, \rho_m}{\sqrt{\rho_i}\; t_r^{eff} + B/b\, \hat{\sigma}\theta(\hat{\sigma})}$$



$$P = 0$$
$$\rho_m = 10^9$$
$$\rho_i = 10^{10}$$
$$B = 0.001\,\text{Poise}$$

- Inverse Kinetic Equation
  - Stress as a function of strain rate, density and temperature
  - Low stresses: $\frac{\hat{\sigma}}{\sigma_c} \approx \left(\frac{\dot{\epsilon}\,\tau\,\sqrt{\rho_i}}{b\,\rho_m}\right)^{1/A^2 \log_{10} e}$
  - High stresses: $\frac{\hat{\sigma}}{\sigma_c} \approx \frac{\dot{\epsilon}}{b\,\rho_m}\left(\sqrt{\rho_i}\, t_B + \frac{B}{b\,\sigma_c}\right)$

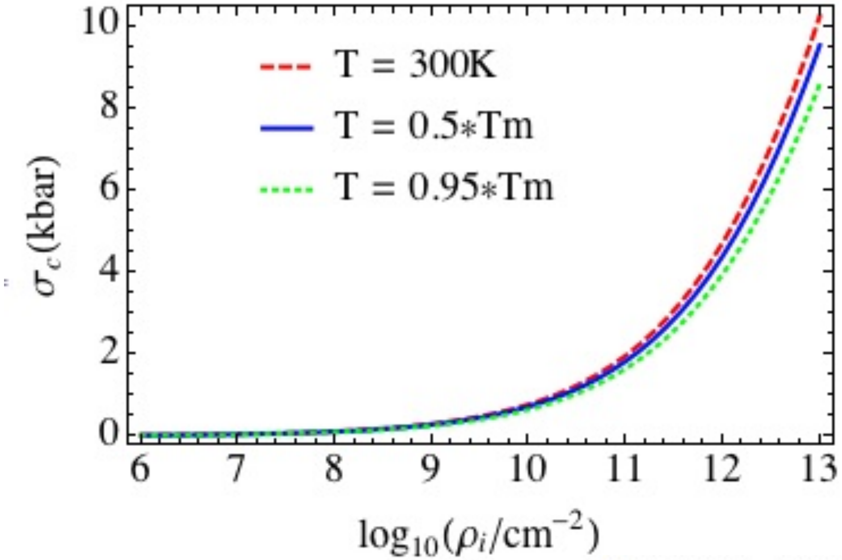
Inverse Kinetic Equation

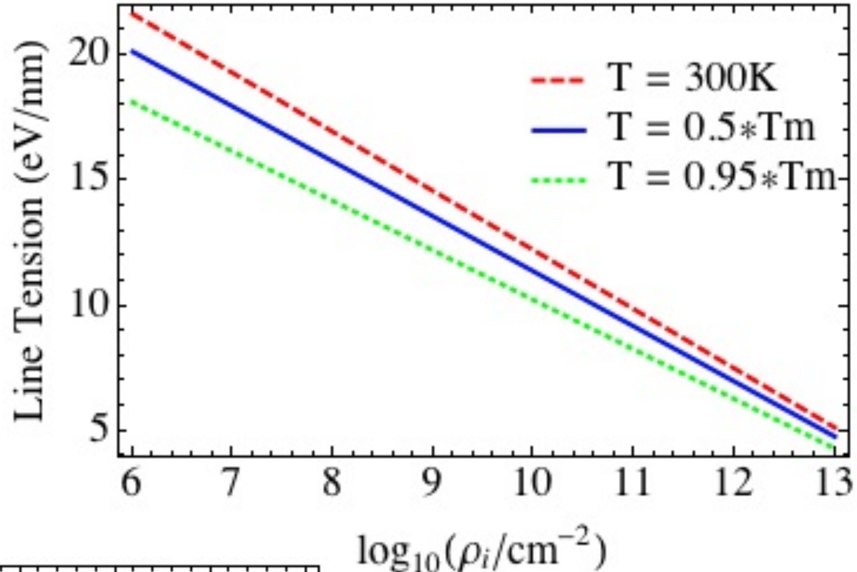


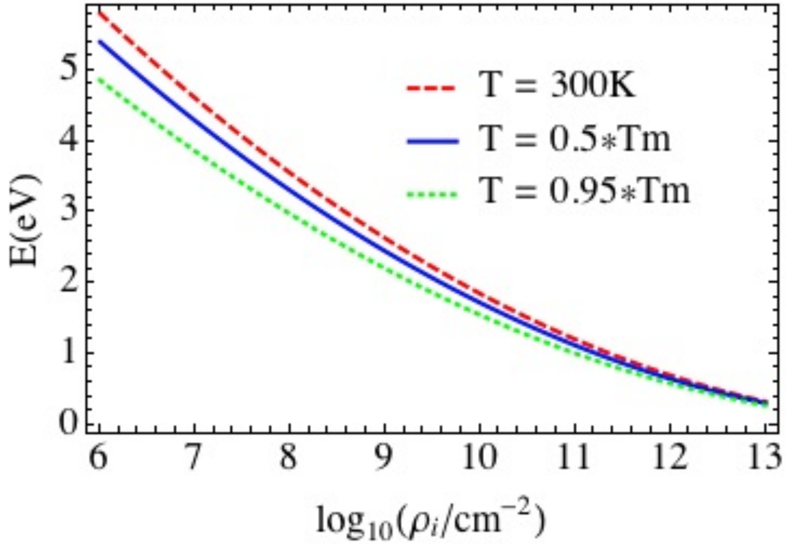
Density and Temperature Dependence

- Shear Modulus: $$G(\rho, T) = G(\rho, 0)\left(1 - \beta\,\frac{T}{T_m(\rho)}\right)$$
- Melt Temperature: $$\frac{d\,\ln T_m(\rho)}{d\,\ln\,\rho} = 2\left(\gamma(\rho) - \frac{1}{3}\right)$$
- Burgers Vector: $$b(\rho) = b(\rho_0)\left(\frac{\rho_0}{\rho}\right)^{1/3}$$
- Dislocation Densities: $$\rho_{m,\,i}(\rho) = \rho_{m,\,i}(\rho_0)\left(\frac{\rho}{\rho_0}\right)^{2/3}$$
- Dislocation Line Tension: $$\mathcal{T}(\rho, T) = \mathcal{T}(\rho_0, T)\left(\frac{\rho_0}{\rho}\right)^{2/3}\frac{G(\rho, T)}{G(\rho_0, T)}$$
- Critical Stress: $$\sigma_c = 2\phi_c\,\mathcal{T}\sqrt{\rho_i}\,/\,b$$
- Activation Energy: $$\mathcal{E}(\rho, T) = \mathcal{E}(\rho_0, T)\,\frac{\rho_0}{\rho}\,\frac{G(\rho, T)}{G(\rho_0, T)}$$

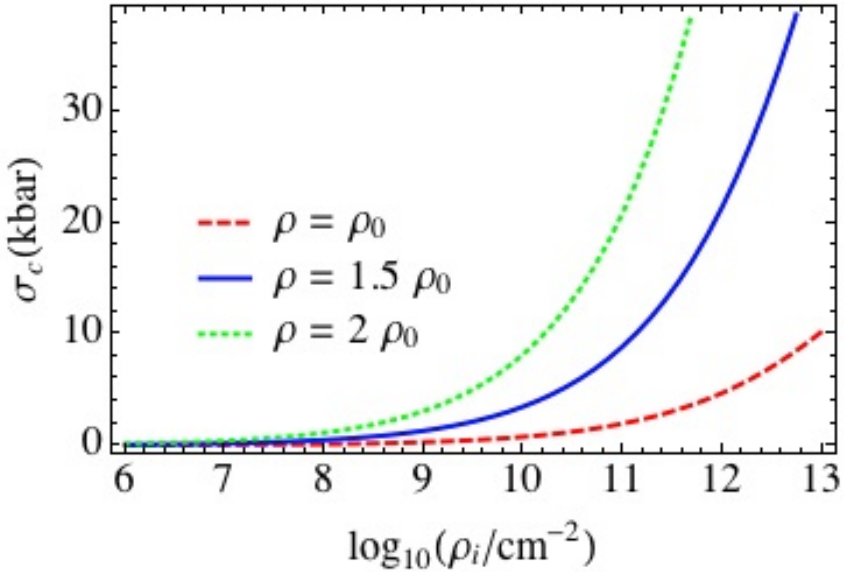
Temperature Dependence

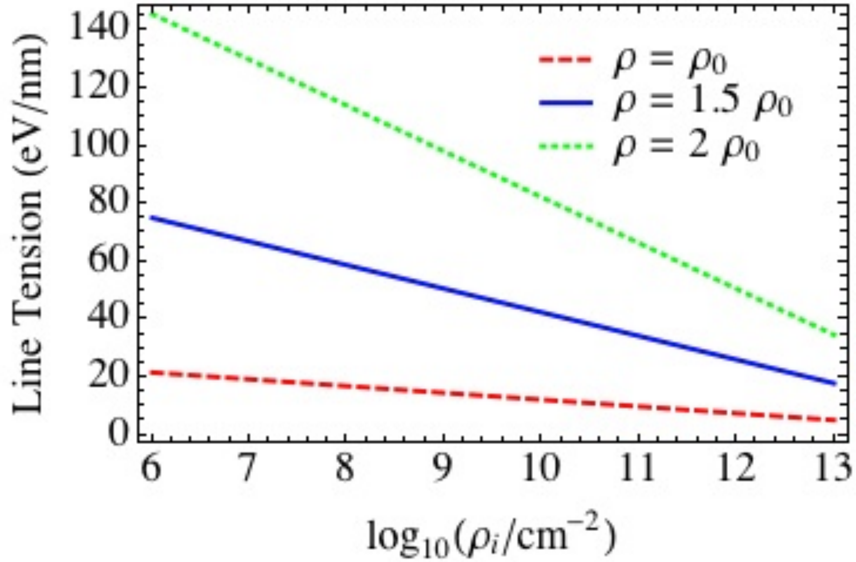


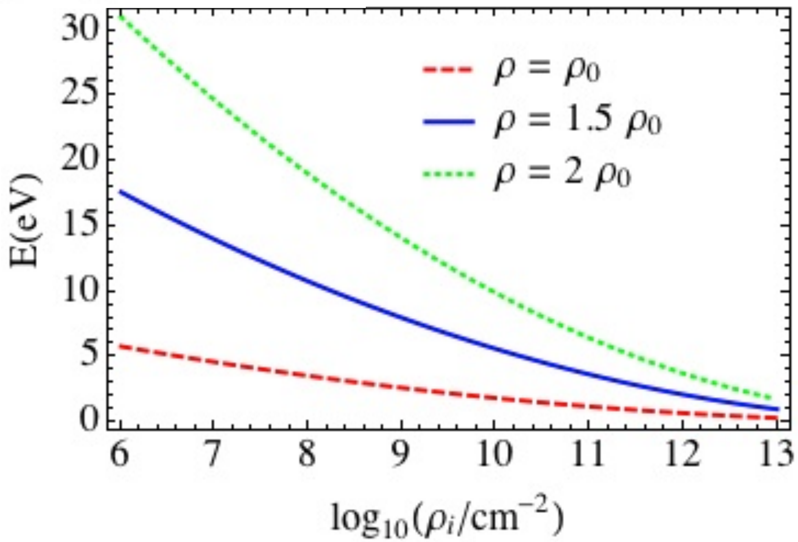




Material Density Dependence

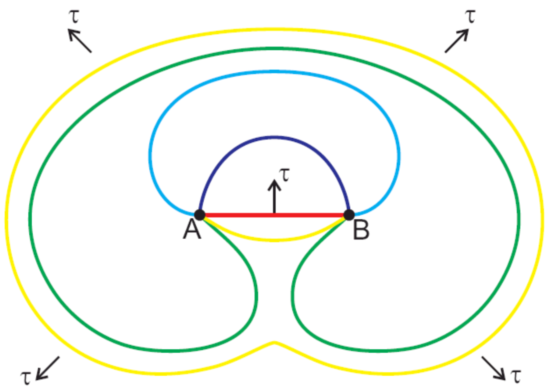




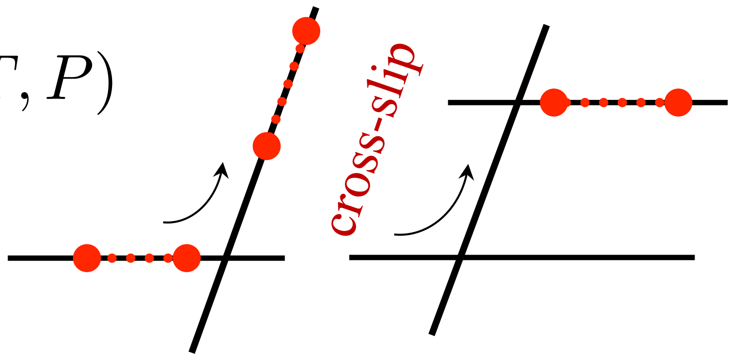


Dislocation Evolution Equations

- Accounts for generation and annihilation of both mobile and immobile dislocation densities through a variety of mechanisms
  - Frank-Read sources
  - Cross-slip
  - Annihilation
    - Mobile - mobile
    - Mobile – immobile
  - Grain boundary nucleation



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



Summary

- Derivation of kinetic equation for high strain rates.
  - Based on MFPT Framework
    - Doesn't break down at high strain rates
  - Accounts for mobile-immobile pairwise dislocation intersections
    - Primary cause of work-hardening in fcc metals
    - Predominant rate-controlling mechanism in fcc metals
  - Account for dissociation with respect to applied forces and thermally-driven force fluctuations.
- Future work
  - Dislocation evolution equations

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Abstract

Describing material strength at very high strain rates is a key component for investigating and predicting material deformation and failure under shock loading. However, accurately describing deformation physics in this strain rate regime remains a challenge due to the break down of fundamental assumptions that apply to material strength at low strain rates. We present a dislocation dynamics model of the plastic flow of fcc polycrystals from quasi-static to very high strain rates (10^6 s^{-1} and above), pressures from ambient to 1000 GPa, and temperatures from zero to melt. The model is comprised of three coupled ordinary differential equations: a kinetic equation, which relates the strain rate to the stress, mobile and immobile dislocation densities, mass density, and temperature, and two equations describing the evolution of the mobile and immobile (network, forest) dislocation densities.

The focus of this presentation is the kinetic equation (evolution equations will be discussed by my collaborator) that accounts for mesoscale deformation behaviors and can be applied to high strain rate regimes without a breakdown of the model framework. Continuum-scale models traditionally have difficulty accounting for specific mesoscale deformation behavior due to the larger length scales (tens to hundreds of microns) at which these models are applicable. In particular, the intersections of attractive dislocations have been shown to be a primary cause of work hardening in metals and a predominant rate-controlling mechanism in fcc metals at low to modest strain rates for temperatures of order 300K and higher[1]. Our kinetic equation describes the formation and dissolution of mobile-immobile dislocation intersections using a mean first passage time (MFPT) framework. By applying MFPT theory to dislocation interactions, deformation mechanics at high strain rates is better described than in traditional models. As part of the derivation, we also determine the probability of dislocation node survival and the mean remobilization time, which is inversely proportional to the strain rate. This equation is designed to describe a number of dislocation interactions over a wide range of strain rates, in particular at rates greater than 10^6 s^{-1}.

[1]J. Friedel, *Dislocations* (Pergamon Press, Oxford, 1964).