Phase-Field theory and modeling of dislocations in ductile single crystals

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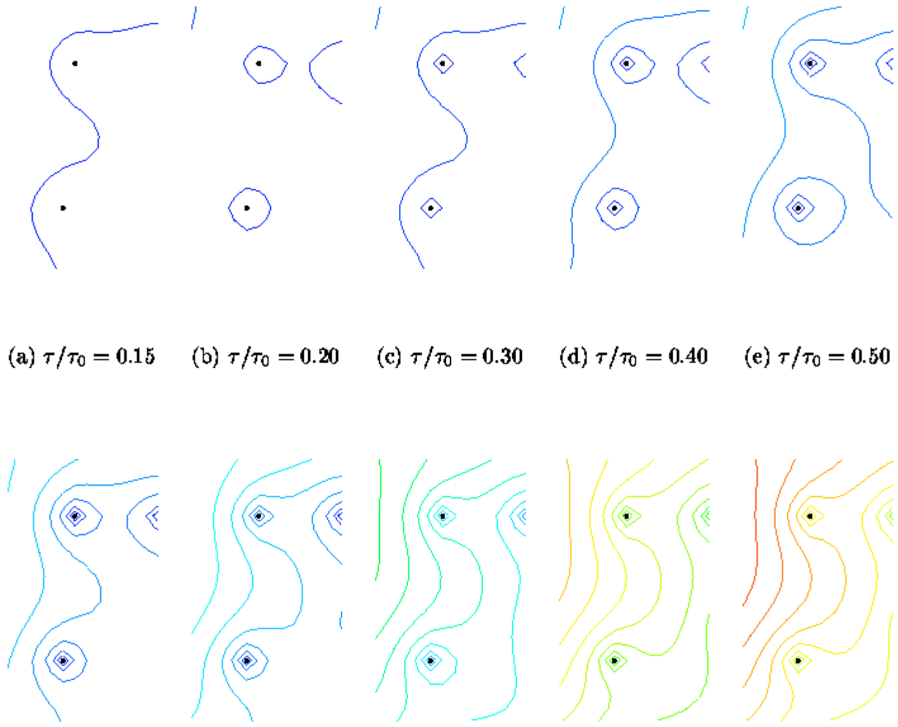
Motivation

- The aim of this study is to develop a phase-field theory of dislocation dynamics, strain hardening and hysteresis in ductile single crystals.

- This representation enables to identify individual dislocation lines and arbitrary dislocation geometries, including tracking intricate topological transitions such as loop nucleation, pinching and the formation of Orowan loops.

- This theory permits the coupling between slip systems, consideration of obstacles of varying strength and anisotropy and thermal effects.

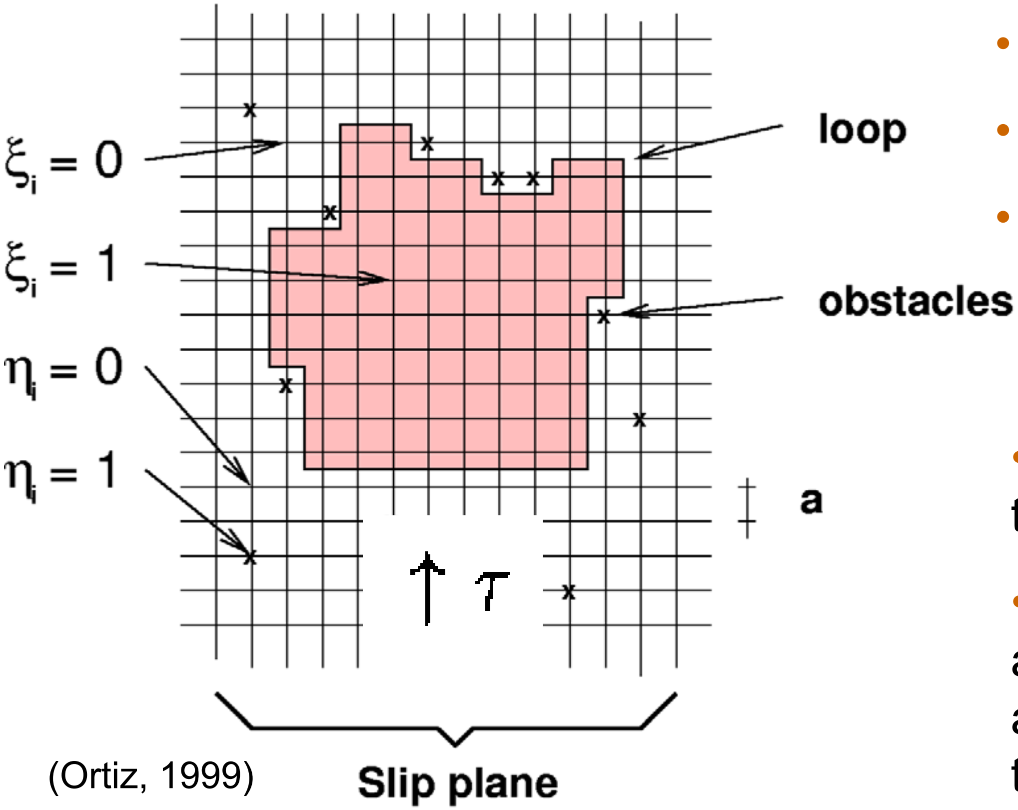
- Rate effects are observed at finite temperatures.



(a) $\tau/\tau_0 = 0.15$ (b) $\tau/\tau_0 = 0.20$ (c) $\tau/\tau_0 = 0.30$ (d) $\tau/\tau_0 = 0.40$ (e) $\tau/\tau_0 = 0.50$

(f) $\tau/\tau_0 = 0.60$ (g) $\tau/\tau_0 = 0.70$ (h) $\tau/\tau_0 = 0.80$ (i) $\tau/\tau_0 = 0.90$ (j) $\tau/\tau_0 = 0.91$ (last step)

Overview



(Ortiz, 1999)

Lattice model of dislocation loop-point obstacle interaction

Effective Dislocation Energy

- Core Energy
- Dislocation Interaction
- Irreversible Obstacle Interaction

Equilibrium configurations

- Closed form solution at zero temperature.
- Metropolis Monte Carlo algorithm and mean field approximation at finite temperatures.

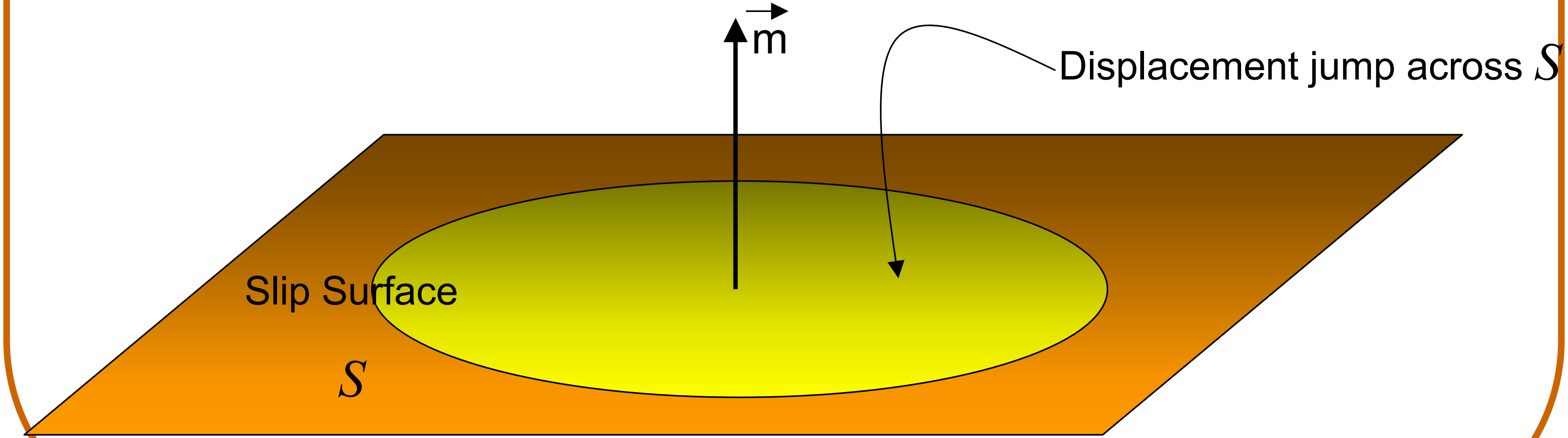
Macroscopic Averages

$$\gamma \propto < \xi > \qquad \rho \propto < \left| \nabla \xi \right| >$$

Effective Energy

$$E[u] = \underbrace{\frac{1}{2}\int c_{ijkl}\beta^e_{ij}\beta^e_{kl}d^3x}_{\text{Elastic interaction}} + \underbrace{\int_S \phi(\delta)dS}_{\text{Core energy}} - \underbrace{\int_S t_i\delta_i dS}_{\text{External field}}$$

where $u_{i,j} = \beta^e_{ij} + \beta^p_{ij}$ with $\beta^p_{ij} = \delta_i m_j \delta_D(S)$



Elastic interaction

$$E^{\text{int}} = \frac{1}{2}\int c_{ijkl}\beta_{ij}^{e}\beta_{kl}^{e}d^{3}x$$

Elastic distortion: $\beta_{kl}^{e} = -G_{ki,l} * \left(c_{ijmn}\beta_{mn}^{p}\right)_{,j} - \beta_{kl}^{p}$

$$\boxed{E^{\text{int}}[\zeta] = \frac{1}{(2\pi)^{2}}\int \frac{\mu b^{2}}{4}K(k_1,k_2)\left|\hat{\zeta}\right|^{2}d^{2}k}$$

with $\zeta(x_1,x_2) = \delta(x_1,x_2)/b$

$$K(k_1,k_2) = \frac{1}{1-\nu}\frac{k_1{}^{2}}{\sqrt{k_1{}^{2}+k_2{}^{2}}} + \frac{k_2{}^{2}}{\sqrt{k_1{}^{2}+k_2{}^{2}}}$$

External Field

$$E^{ext} = \int_S \delta_i t_i dS$$

with: $\delta_i(x_1,x_2) = \zeta(x_1,x_2) b_i$

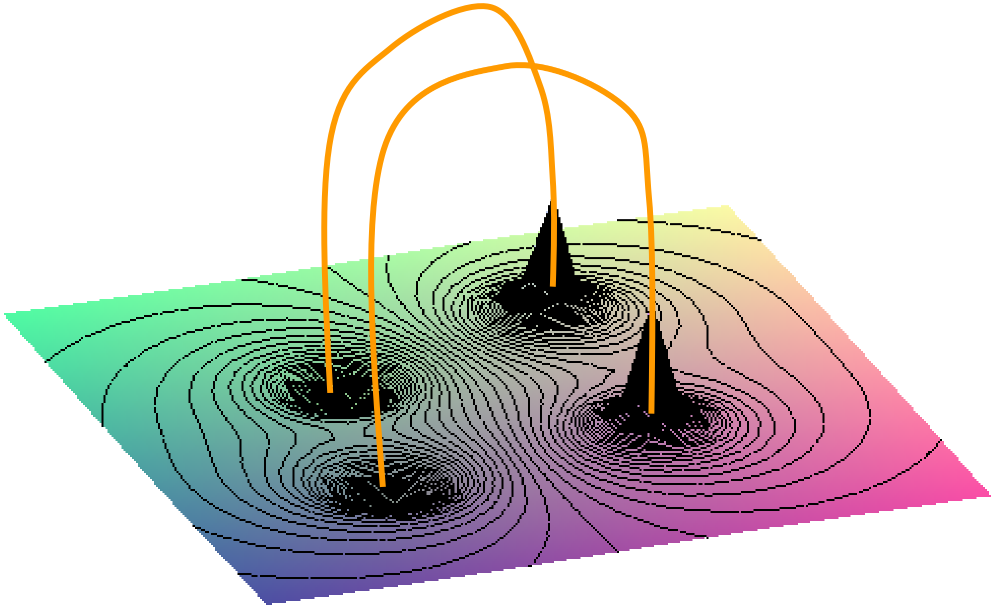
$$s(x_1,x_2) = t_i(x_1,x_2) b_i$$

$$s(x) = \tau + \sum_{n=1}^{Ndis} \frac{C_n}{\left|x - x_n\right|}$$

applied

shear stress

forest dislocations



$$\boxed{E^{ext} = \int_S bs\zeta dS}$$

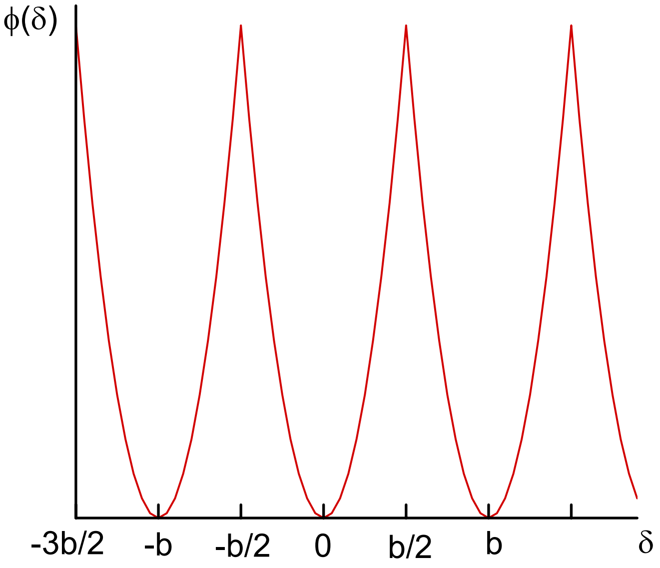
Core Energy

$$\phi(\delta) = \min_{\xi \in Z} \frac{1}{2} C_{ij} \left(\delta_i - \xi b_i\right)\left(\delta_j - \xi b_j\right)$$

$$\xi : S \to Z \qquad\qquad C_{ij} = \frac{\mu}{2d}\delta_{ij}$$

$$\downarrow$$

$$\phi(\zeta) = \inf_{\xi \in Z} \frac{b^2 \mu}{4d} \left|\zeta - \xi\right|^2$$



Ortiz and Phillips, 1999

$$\boxed{E^{core} = \int_S \phi(\zeta)\, dS}$$

Phase-Field Energy

$$E[\xi] = \inf_{\zeta \in Y} \frac{1}{(2\pi)^2} \int \left(\frac{\mu b^2}{2d} \left| \hat{\zeta} - \hat{\xi} \right|^2 + \frac{\mu b^2}{4} K \left| \hat{\zeta} \right|^2 - b \hat{s}^* \hat{\zeta} \right) d^2 k$$

Minimization with respect to ζ gives:

$$\hat{\zeta} = \frac{d}{\mu b} \frac{\hat{s}}{1 + Kd/2} + \frac{\hat{\xi}}{1 + Kd/2}$$

core regularization factor

$$\boxed{E[\xi] = \frac{1}{(2\pi)^2} \left[\int \frac{\mu b^2}{4} \frac{K}{1 + Kd/2} \left| \hat{\xi} \right|^2 d^2 k - \int \frac{b \hat{s}^* \hat{\xi}}{1 + Kd/2} d^2 k \right] + E_0}$$

elastic energy

Phase-Field Energy

Elastic energy

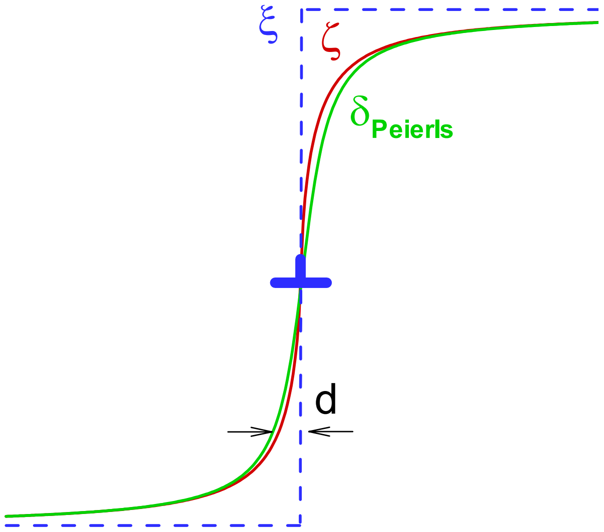
$$E_0 = \frac{1}{(2\pi)^2}\int \frac{d}{2\mu}\frac{\left|\hat{s}\right|^2}{1+K^{d/2}}\, d^2k$$

Core regularization

$$\zeta = \zeta_0 + \varphi_d * \xi$$

Core regularization factor

$$\hat{\varphi}_d(k) = \frac{1}{1+K^{d/2}}$$



$$\delta_{Peierls} = -\frac{b}{2\pi}\tan^{-1}\frac{2(1-\nu)x}{d}$$

Irreversible Process and Kinetics

- Irreversible dislocation-obstacle interaction may be built into a variational framework, we introduce the incremental work function:

$$W[\xi^{n+1} \mid \xi^{n}] = E[\xi^{n+1}] - E[\xi^{n}] + \underbrace{\int f(x) \left| \xi^{n+1} - \xi^{n} \right| d^{2}x}_{\text{incremental work dissipated at the obstacles}}$$

- Primary and forest dislocations react to form a jog: $f \propto \frac{\mu b^{2}}{4\pi}$
- Updated phase-field follows from: $\inf_{\xi_{n+1} \in X} W[\xi^{n+1} \mid \xi^{n}]$
- Short range obstacles: $f(x) = b\tau^{P} + \sum_{i=1}^{N} f_{i} \varphi_{d}(x - x_{i})$

Irreversible Process and Kinetics

$$\int f(x)\left|\zeta^{n+1}-\zeta^{n}\right|d^{2}x=\sup_{\left|g^{n+1}\right|\leq f}\int g^{n+1}(x)\left(\zeta^{n+1}-\zeta^{n}\right)d^{2}x$$

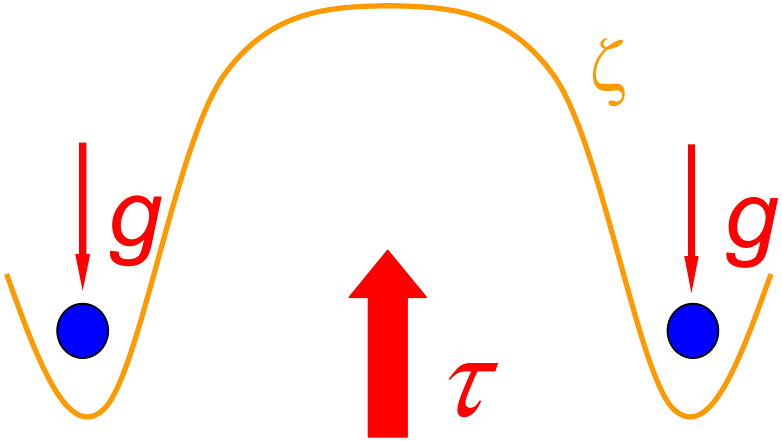
Kuhn-Tucker optimality conditions:

$$\xi_i^{n+1}-\xi_i^{n}=\lambda_i^{+}-\lambda_i^{-}$$

$$g_i^{n+1}-f_i\leq 0 \qquad -g_i^{n+1}-f_i\leq 0$$

$$\lambda_i^{+}\geq 0 \qquad \lambda_i^{-}\geq 0$$

$$\left(g_i^{n+1}-f_i\right)\lambda_i^{+}=0 \qquad \left(g_i^{n+1}+f_i\right)\lambda_i^{-}=0$$



Equilibrium condition:

$$b\,\tau^{n+1}=\frac{1}{\Omega}\sum_{i=1}^{N}g_i^{n+1}$$

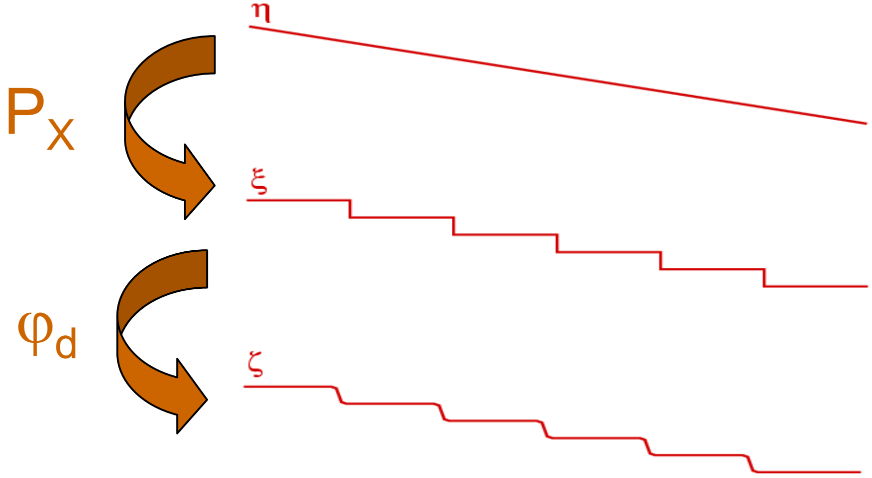
Energy minimizing phase-field

Unconstrained minimization problem: $\inf_{\eta \in Y} W[\eta] \longrightarrow \frac{\mu b}{2} K \hat{\eta} = \hat{s}$

if $\langle s \rangle = 0$ $\boxed{\eta = G * s + C}$

with $$G(x) = \frac{2}{\mu b} \int \frac{e^{ik \cdot x}}{(2\pi)^2 K} d^2 k = \frac{1}{(\mu b \pi)} \frac{\sqrt{x_1^2 + x_2^2}}{x_1^2 + x_2^2/(1-\nu)}$$

$$\boxed{\zeta = \varphi_d * P_X\left(G * s\right) + C}$$

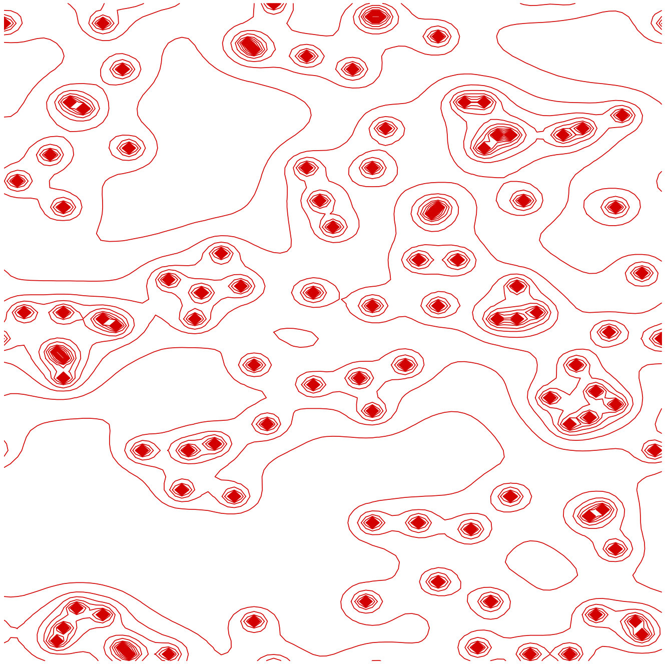


Closed-form solution

$$\eta_i^{n+1} = -\sum_{j=1}^{N} G_{ij} g_j^{n+1} + C^{n+1}$$

$$G_{ij} = G(x_i - x_j)$$

$$G_{ii} = \frac{(2-\nu)\sqrt{1-\nu}}{2\pi^2 b\mu}\frac{1}{d}$$



Dislocation loops

Macroscopic averages

- Slip

$$\gamma = \frac{b}{lN}\sum_{i=1}^{N}\xi_i = \gamma_0\langle\xi\rangle \qquad l \approx 10^3 b$$

- Dislocation density

$$\rho = \rho_0 b\langle|\nabla\xi|\rangle \qquad \rho_0 = \frac{1}{bl} \approx 10^{16}\frac{1}{m^2}$$

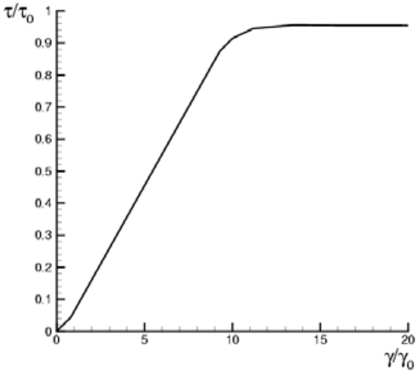
- Obstacle concentration

$$c = \langle\eta\rangle \qquad c \approx 10^{12} - 10^{17}\frac{1}{m^2}$$

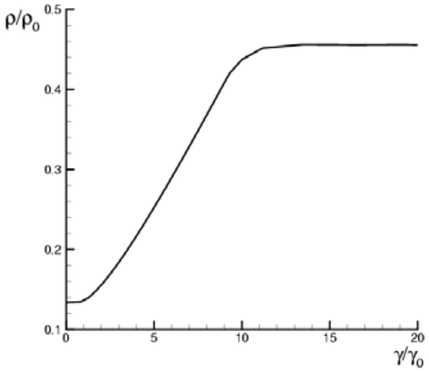
- Shear stress

$$\tau = \tau_0\frac{\langle f\rangle}{\langle F^{obs}\rangle} \qquad \tau_0 = F^{obs}c \approx 10^{-2} - 10^{-4}\mu$$

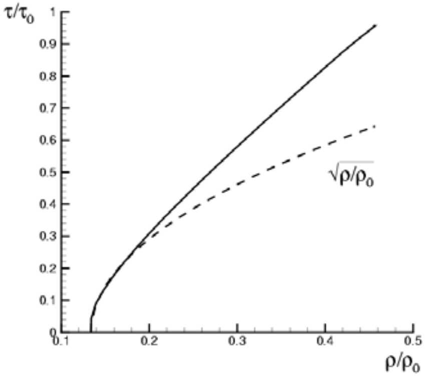
Monotonic loading



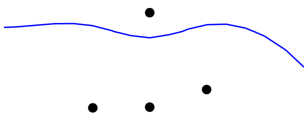
Stress-strain curve.



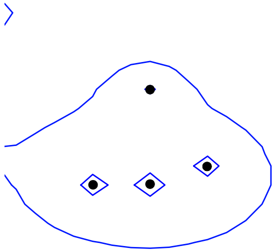
Evolution of dislocation density with strain.



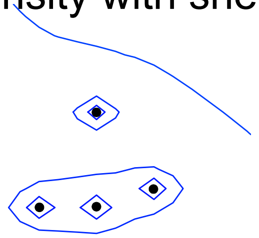
Evolution of dislocation density with shear stress.



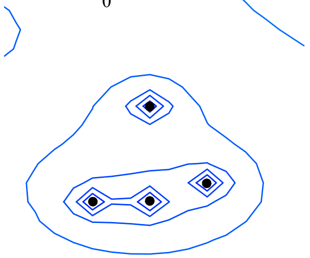
$\tau / \tau_0 = 0.00$



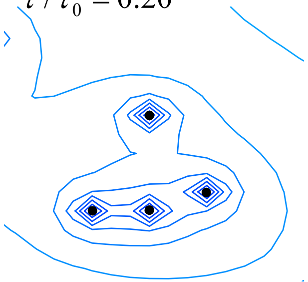
$\tau / \tau_0 = 0.20$



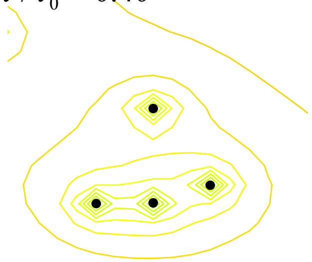
$\tau / \tau_0 = 0.40$



$\tau / \tau_0 = 0.60$

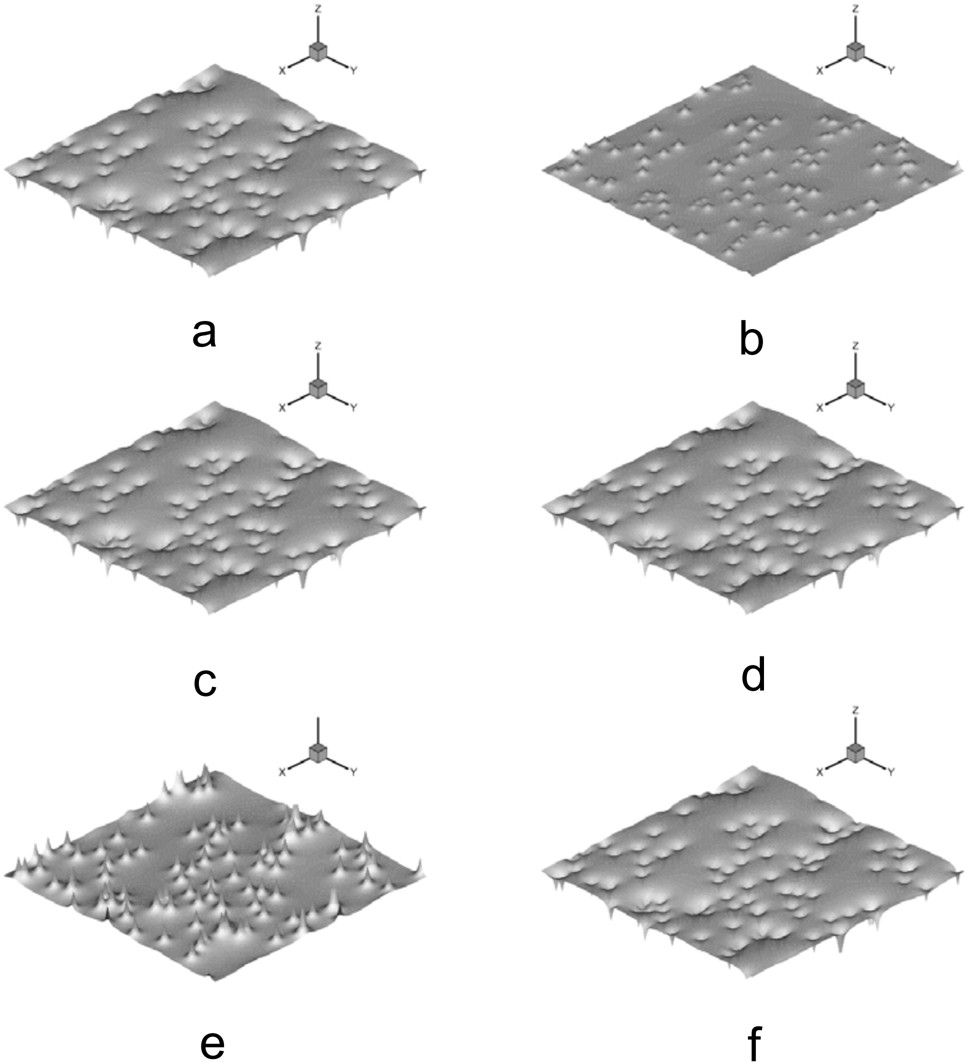


$\tau / \tau_0 = 0.80$

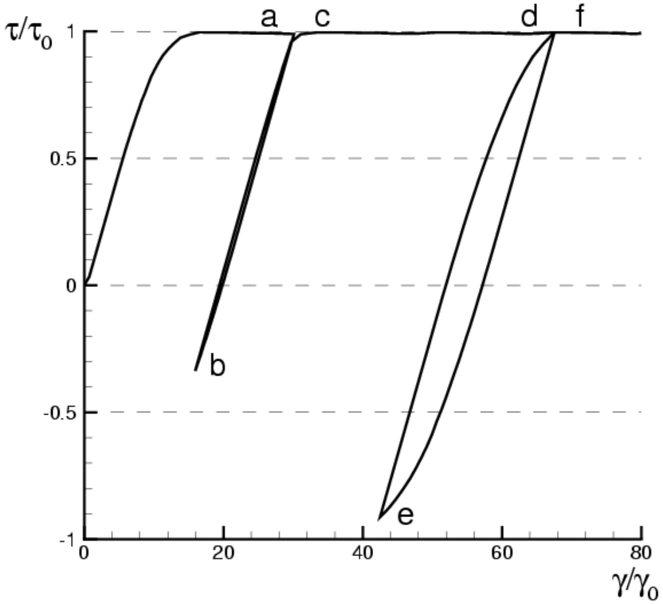


$\tau / \tau_0 = 0.99$

Fading memory

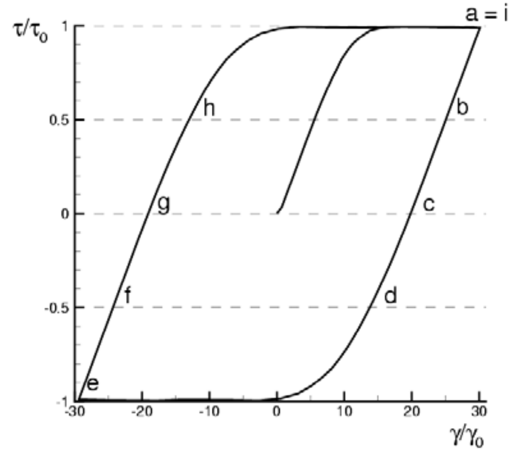


Three dimensional view of the evolution of the phase-field, showing the the switching of the cusps.

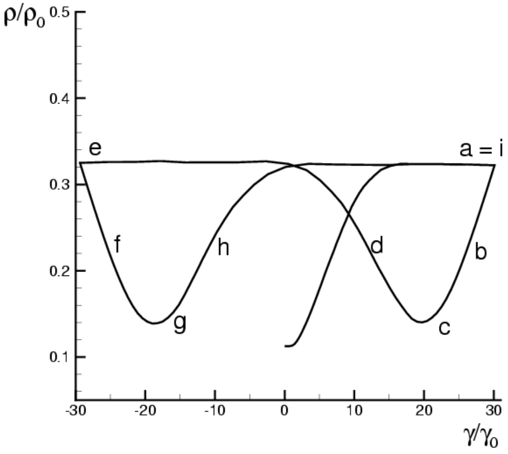


Stress-strain curve.

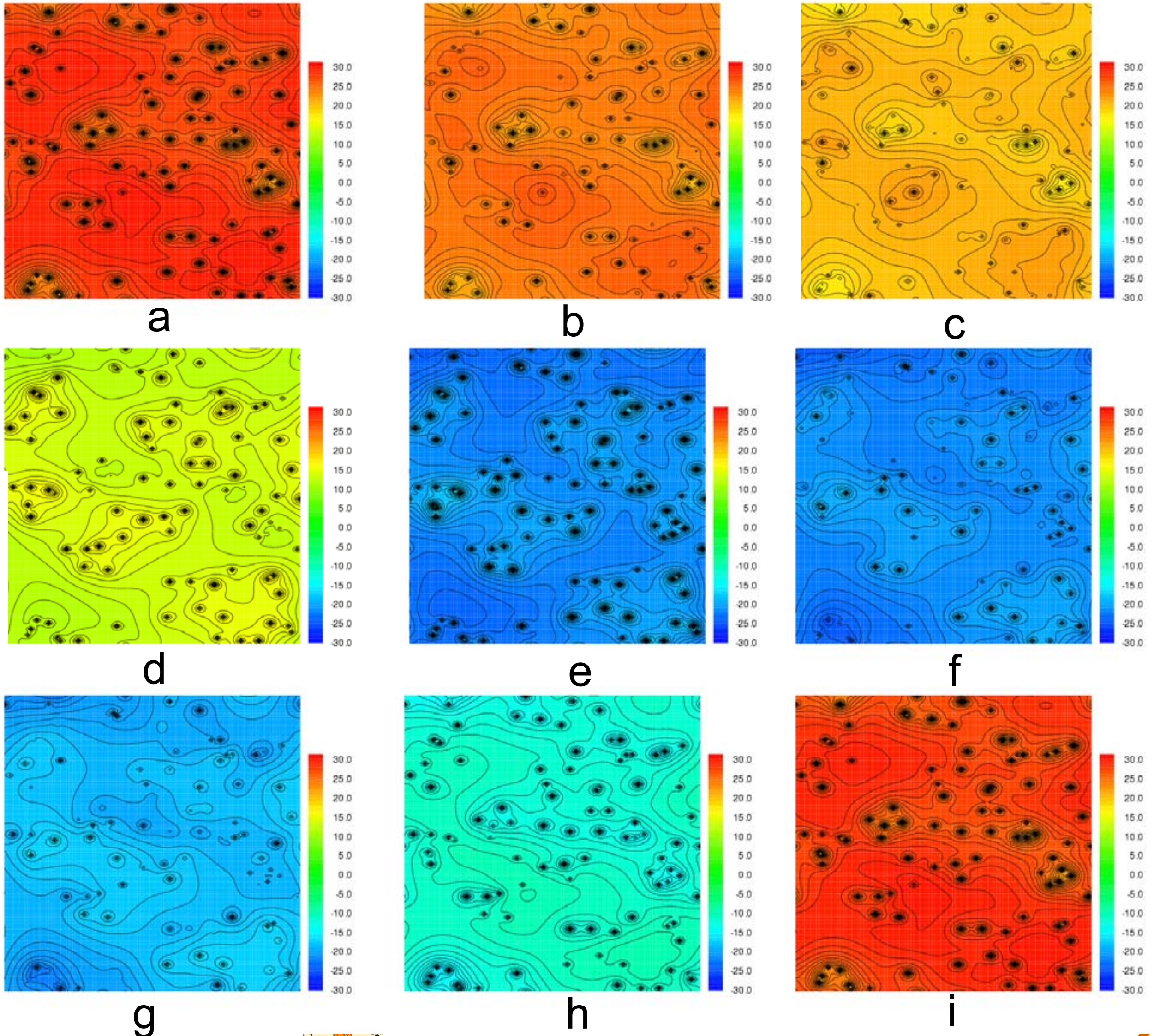
Cyclic loading



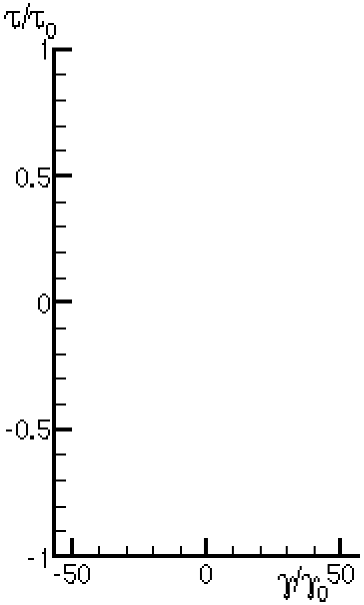
Stress-strain curve.

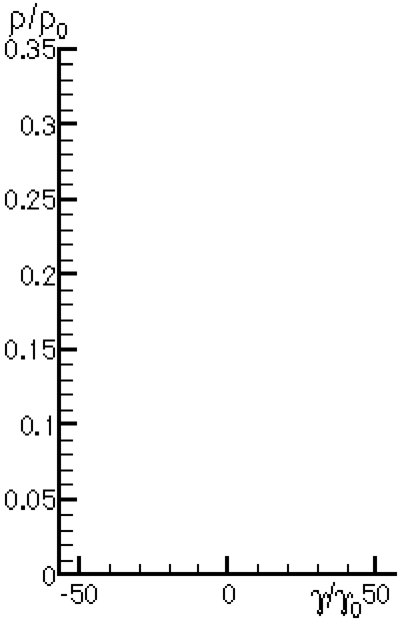


Evolution of dislocation density with strain.

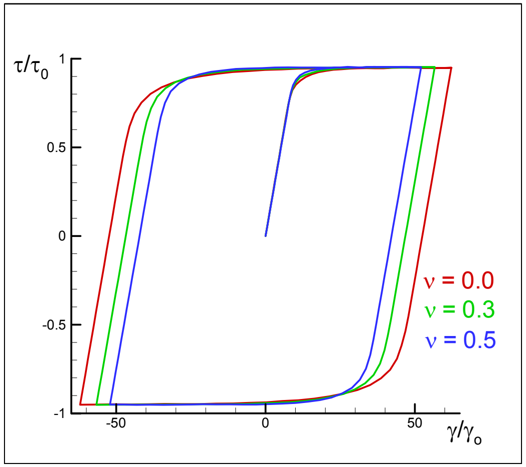


Cyclic loading

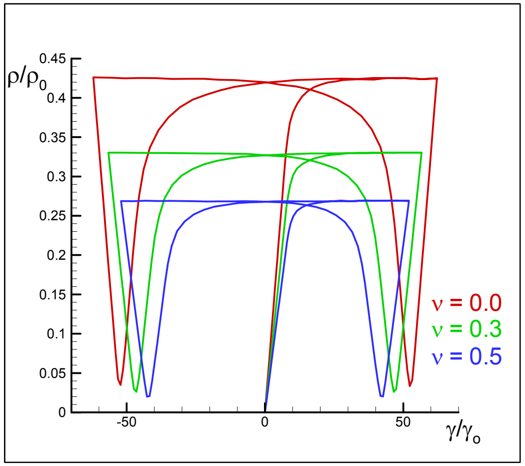




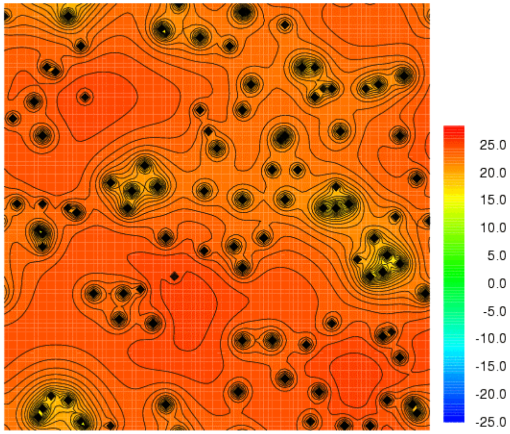
Poisson ratio effects



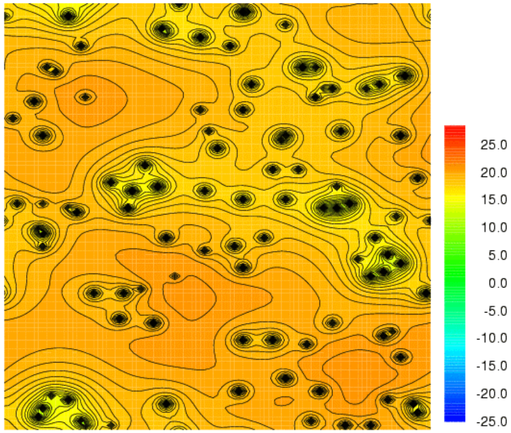
Stress-strain curve.



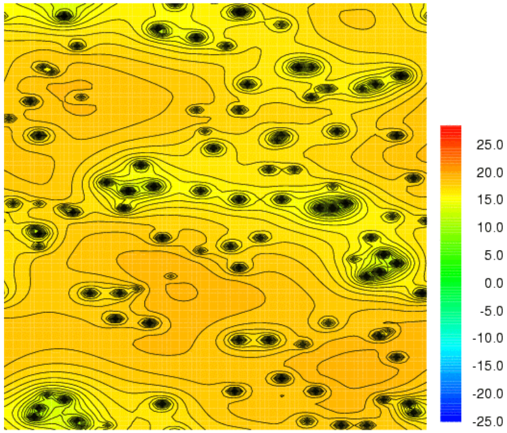
Evolution of dislocation density with strain.



$$\nu = 0.0$$

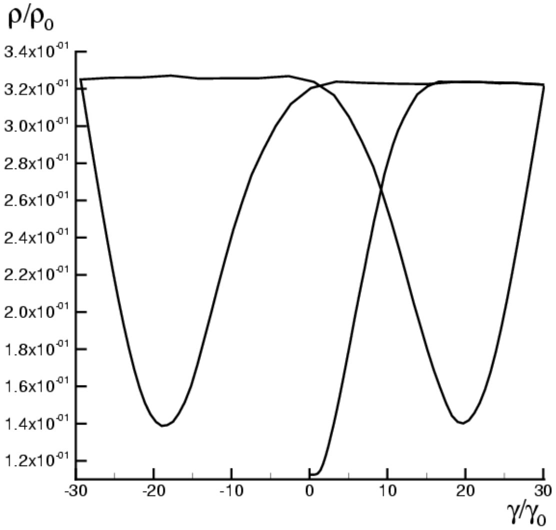


$$\nu = 0.3$$

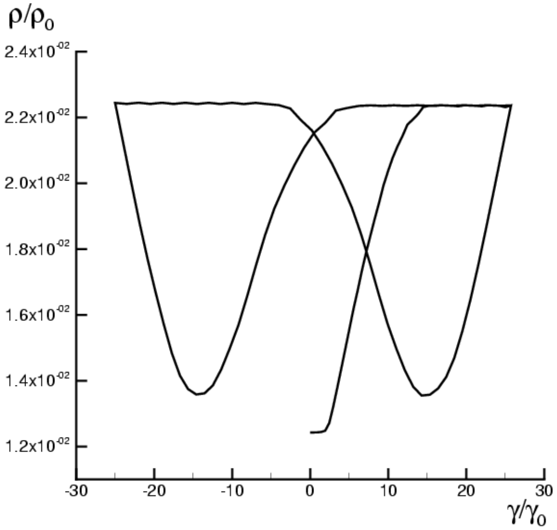


$$\nu = 0.5$$

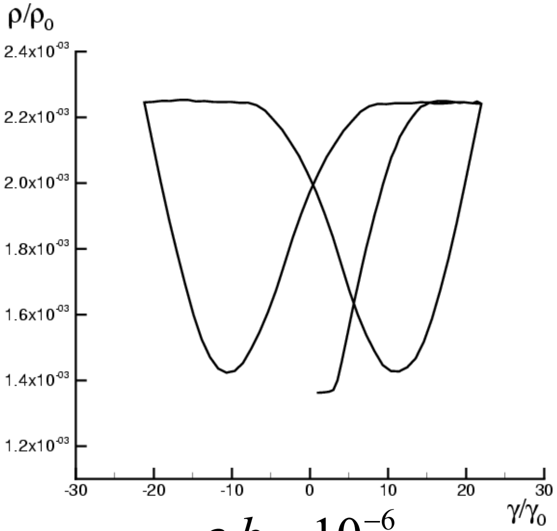
Obstacle density



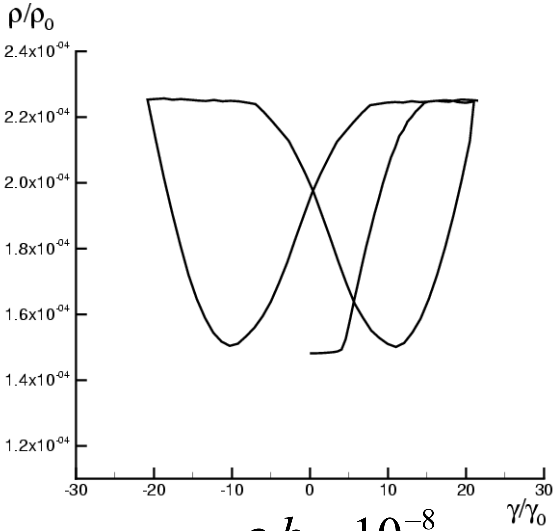
$\rho\, b = 10^{-2}$



$\rho\, b = 10^{-4}$



$\rho\, b = 10^{-6}$



$\rho\, b = 10^{-8}$

Temperature effects

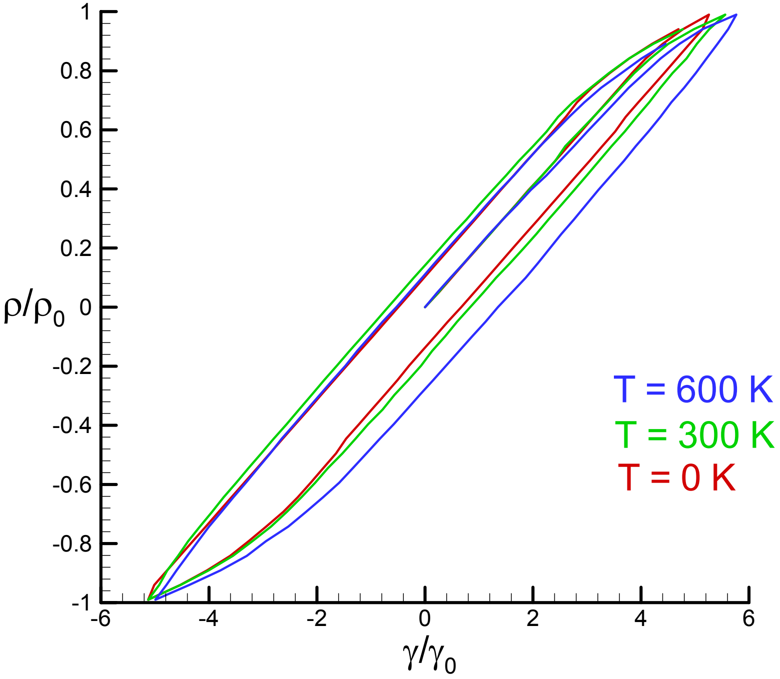
- Incremental work function

$$W[\xi^{n+1} \mid \xi^{n}] = E[\xi^{n+1}] - E[\xi^{n}] + \underbrace{\sum_{i=1}^{Nobs} F_i^{obs} \left|\xi^{n+1} - \xi^{n}\right|}_{\text{incremental work dissipated at the obstacles}}$$

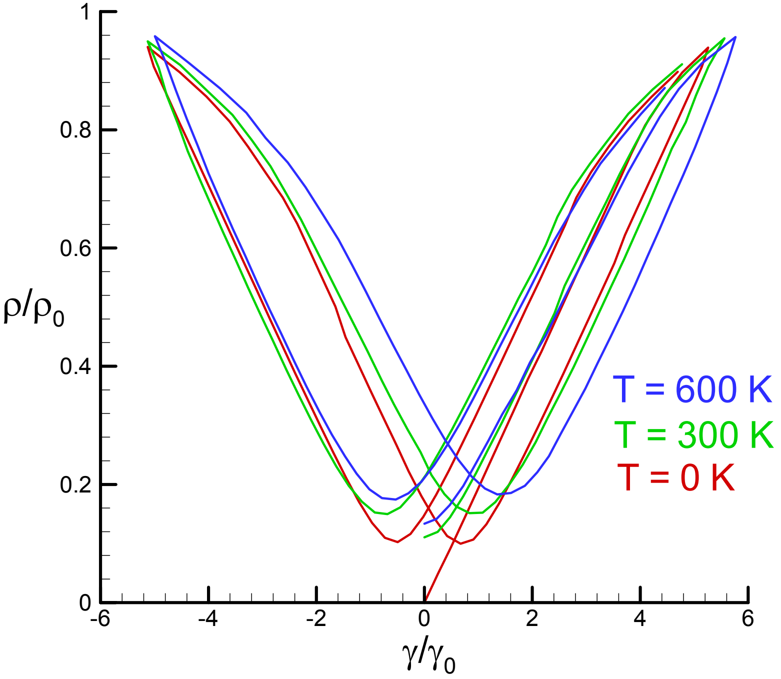
- Metropolis Monte Carlo algorithm with hysteresis.
- Dislocation interaction is calculated in Fourier transformed space.

$$\mu = 5.6 \cdot 10^{10}\, Pa \qquad b = 2.5 \cdot 10^{-10}\, m$$

Temperature Effects



Stress-strain curve.

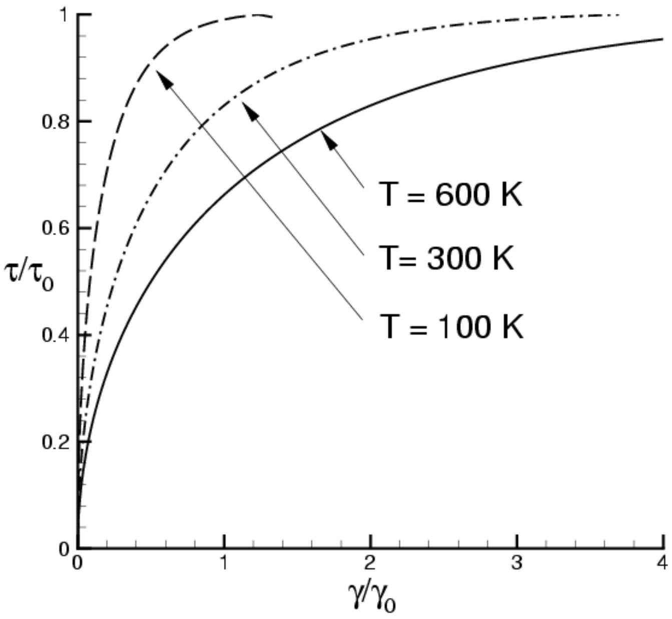


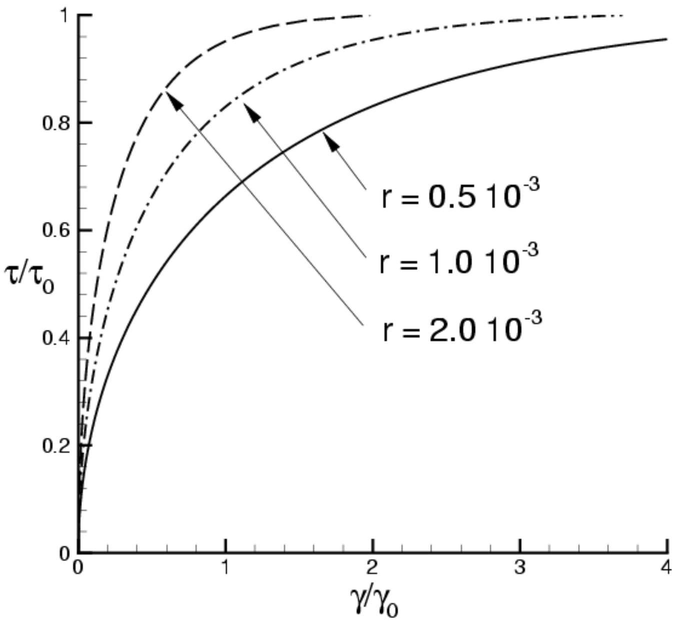
Evolution of dislocation density with strain.

Mean field approximation

$$\Delta w(\gamma_{n+1},\gamma_n) = b^3\left[-\tau_{n+1}\gamma_{n+1} + \tau_n\gamma_n + \tau_0\left|\gamma_{n+1} - \gamma_n\right|\right]$$

$$\left\langle\gamma_{n+1}\right\rangle = \left\langle\gamma_n\right\rangle + \frac{2\tau_{n+1}}{\beta b^3(\tau_0^2 - \tau_{n+1}{}^2)}$$

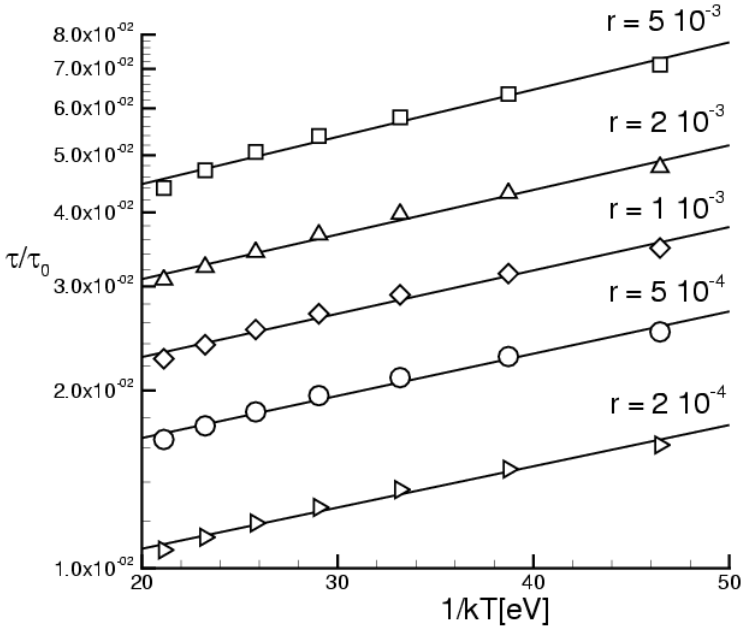




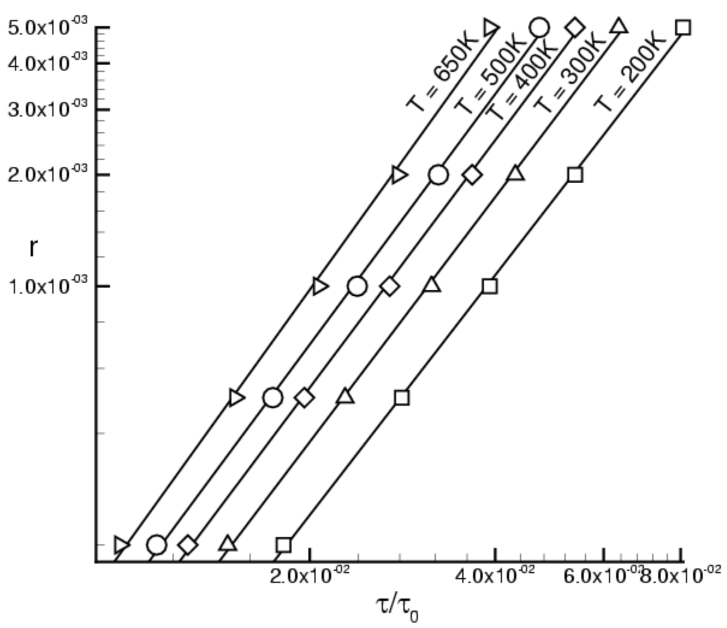
Mean field approximation

$$r = A\left(\frac{\tau}{\tau_0}\right)^n \exp\left(-\frac{U}{kT}\right)$$

(Kocks, Argon, Ashby, 1975)



Flow stress vs. temperature



Deformation rate vs. flow stress

Conclusions

- The phase-field representation furnishes a simple and effective means of tracking the motion of large numbers of dislocations within discrete slip planes through random arrays of obstacles (forest dislocations, defects) under the action of an applied shear stress.
- The theory predicts a range of behaviors which are in qualitative agreement with observation, Bauschinger effect, formation of Orowan loops.
- Softening and yield stress dependence on the temperature are observed.
- Rate effects are observed at finite temperature.