Multiscale modeling of plastic deformation
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Atomistics: properties of individual defects

Generalized stacking fault energy

\[ E^{\text{SSF}} = \frac{1}{2} \int \left( \sum_{\alpha} \sin^2(n_{\alpha} \xi(x,y)) \right) d^2x \]

Energy required to rigidly slide a block of material (\( \gamma \) surface or generalized stacking fault energy) Parameter A: unstable stacking fault (USF) energy

Dislocation core energies

\[ E^{\text{prod}} = \frac{1}{2} \int \sum_{\alpha} \frac{H(\alpha, x) \partial(\xi(x,y))}{\partial x} \frac{\partial(\xi(x,y))}{\partial d} d^3x \]

Tensor \( H \) from dislocation core energies (\( E_C \))

Phase-Field MicroMechanics

Plastic deformation gradient

\[ \gamma(x) = \frac{1}{2} \sum_{\alpha} \xi(x, y) = \alpha \theta(x, y) \]

Time evolution follows Ginsburg-Landau equation

\[ \frac{\partial \xi(x,y)}{\partial t} = -\frac{\partial E}{\partial \xi(x,y)} \]

Total energy

\[ E = E^{\text{eff}} + E^{\text{SSF}} \]

From atomic simulations of single crystal Ni

\[ E^{\text{eff}} = \frac{1}{2} \sum_{\alpha} \left( \frac{\partial^2 E}{\partial \xi^2} \right) \left( \frac{\partial \xi}{\partial \theta} \right)^2 \]

From simulations: Gamma surface

\[ E^{\text{eff}} = \frac{1}{2} \sum_{\alpha} \left( \frac{\partial^2 E}{\partial \xi^2} \right) \left( \frac{\partial \xi}{\partial \theta} \right)^2 \]

From simulations: Core energy

\[ E^{\text{eff}} = \frac{1}{2} \sum_{\alpha} \left( \frac{\partial^2 E}{\partial \xi^2} \right) \left( \frac{\partial \xi}{\partial \theta} \right)^2 \]

To Continuum

Strain hardening

\[ \sigma_{yy} = \sigma_{0}(t, \theta) + \sigma_{y}(t, \theta, \rho) \]

- Grain size effects
- Deviation of the average grain size affects hardening and Bauschinger effect.

Plasticity occurs when effective stress is above yield close up view of effective plastic strain

\[ \dot{\gamma} = h(\rho) \dot{\rho} \]

\[ \rho = \rho(\dot{\epsilon}, \rho_0, \rho_{\text{sat}}) \]

\[ \rho(\dot{\epsilon}, \theta, \tau) = c \frac{\rho_{\text{sat}}}{\sqrt{1 - \frac{1}{2} (1 - \frac{1}{2})^2 + \rho_0}} \]

\[ h(\rho) = \alpha b \sqrt{\rho} \]

MPM

\[ \rho \frac{d\dot{\epsilon}}{dt} = \dot{\epsilon}^{\text{int}} + \dot{\epsilon}^{\text{ext}} \]

\[ \dot{\epsilon}^{\text{int}} = -\nabla \cdot \sigma \]

\[ \sigma = \sigma_0 \left( \epsilon - \epsilon^p \right) \]

Elastic moduli \( \tilde{C} \) from MD for single crystal plus homogenization to account for texture in the device microstructure

Plasticity determined from von Mises model

\[ E^{\text{VM}} < \sigma \]

defines elastic region

\[ E^{\text{VM}} = \sigma \]

plastic response

\[ \sigma^{\text{VM}} = \frac{1}{2} \sigma : \sigma^{\text{VM}} \]

In the elastic regime, the plastic strain rate is zero, \( \dot{\epsilon}^p = 0 \)

In the plastic regime, the plastic strains are determined from the above with

\[ \dot{\lambda} \geq 0 \]

\[ E^{\text{VM}} < \lambda \dot{E}^{\text{VM}} = 0 \]

The yield stress \( \sigma_y \) is determined from PFMM

Ni membrane is 3µm thick and deforms 3µm to open the switch (Half of the membrane is modeled with symmetry on the left)