Comparison of 3D phase field and Peierls-Nabarro modeling of dislocation dissociation, glide and twinning in fcc systems

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• introduction
  • dislocation modeling approaches
  • Voltera, Peierls-Nabarro (PN), phase field (PF)

• PF & PN formulations
  • energy densities
  • stacking fault energy (SFE)
  • interface energy scaling

• results
  • comparison of dissociation in PF & PN
  • dislocation loops under loading
  • twinning vs. glide plasticity

• summary / outlook
dislocation (line) modeling

- molecular dynamics (MD)
  - ideals, partials, SFs resolved
  - finite physical core
  - interatomic potential

- phase field, Peierls-Nabarro
  - ideals, partials, SFs, twins resolved
  - finite physical core
  - non-local thermodynamics

- discrete dislocation dynamics
  - ideals resolved (partials?, SFs?)
  - core negligible / neglected
  - non-local mechanics (elasticity)

- continuum dislocation dynamics

(paradis.stanford.edu)
Volterra & Peierls-Nabarro / phase field

Volterra (V)
\[ u_x \left( 0 \right) = b \rightarrow u_x^+ \left( x \right) \]
\[ \phi^V \left( x \right) \]
\[ x, y = 0^\pm \]

Peierls-Nabarro (PN), phase field (PF)
\[ \phi^{PN} \left( x \right) \]
\[ \phi^{PF} \left( x \right) \]
\[ y = +d/2 \]
\[ y = -d/2 \]
\[ x, y = 0^\pm \]

(e.g., Eshelby, 1949; Peierls, 1949, Nabarro, 1955; Hirth, Lothe, 1982; Schoeck, 1999; Bulatov & Cai, 2006...)
1D comparison core region

• models
  • Peierls-Nabarro (Frenkel; red)
  • phase field (double well; green)
  • Volterra (blue)

\[
\phi^{\text{PN}}(x) = \frac{1}{2} + \frac{1}{\pi} \tan^{-1} \frac{x}{c}
\]

\[
\phi^{\text{PF}}(x) = \frac{1}{2} + \frac{1}{2} \tanh^{-1} \frac{x}{\sqrt{2} c}
\]

\[
k = \frac{\mu b/c}{2\pi(1 - \nu)}
\]

\[
c = \frac{d}{2(1 - \nu)}
\]
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3D Peierls-Nabarro & phase field

- three-dimensional non-local microelasticity

- (generalized) Peierls-Nabarro (PN)
  - two-dimensional disregistry fields (slip planes)
  - free energy: elastic + homogeneous SFE (rigid slip)

\[ \psi(\nabla u, \phi) = \psi_E(\nabla u, \phi) + \psi_H(\phi) \]

  elastic  \quad SFE

- phase field
  - three-dimensional phase fields (slip planes)
  - free energy: elastic + homogeneous SFE + core (non-rigid slip)

\[ \psi(\nabla u, \phi, \nabla \phi) = \psi_E(\nabla u, \phi) + \psi_H(\phi) + \psi_G(\nabla \phi) \]

  elastic  \quad SFE  \quad core

(e.g., Shen, Wang, 2004; Xiang et al., 2008; Hunter et al., 2011, 2013; Mianroodi & Svendsen, 2014…)

application to dislocation lines

- dislocation line $\rightarrow$ residual distortion field

- residual distortion field
  - phase fields ($\phi = 0$ un-slipped $\rightarrow$ $\phi = 1$ slipped)
  - constant distortion system tensors

- elastic free energy density
  $$\psi_E = \frac{1}{2} (E - E_R) \cdot C_E (E - E_R)$$

- strain field
  $$E = \text{sym} \nabla u$$

- stress field
  $$T = \partial_E \psi_E = C_E (E - E_R)$$

- mechanical equilibrium
  $$\text{div} \ T = 0$$

- relaxational dynamics (TDGL)
  $$\dot{\phi}_a = -m_a \delta_{\phi_a} \psi$$

(e.g., Eshelby, 1970; Khachaturyan et al., 1995; Wang et al., 2001; Bulatov & Cai, 2006; …)
homogeneous part / SFE

• two phase fields per \{111\} plane
  • example (111): \((\phi_1, \phi_2) = (\phi_{[\bar{1}10]}, \phi_{[\bar{1}\bar{1}2]})\)

• SFE \{111\} \(\psi_H(\phi_1, \phi_2)\)
  • “parameterized” by \((\phi_1, \phi_2)\)
  • calculated directly from MD / DFT

\[\psi_H(\phi_1, \phi_2)\]

\[\phi_2 \equiv \phi_{[\bar{1}\bar{1}2]}\]
\[\phi_1 \equiv \phi_{[\bar{1}10]}\]

• twinning (PF)
  • phase fields 3d
  • z-dependence \(\langle 111 \rangle\)

(Mianroodi & Svendsen, 2014)
gradient part / core energy

• gradient energy measures (Helmholtz split)
  • glide \[ |\text{curl } H_R|^2 = \sum_{a,b} \nabla \phi_a \cdot N_{ab}^g \nabla \phi_b \]
  • climb \[ |\text{div } H_R|^2 = \sum_{a,b} \nabla \phi_a \cdot N_{ab}^c \nabla \phi_b \]

• gradient moduli based on \( H_a = \gamma_a s_a \otimes n_a, \gamma_a := b_a / d_a \)
  • glide \[ N_{ab}^g = \gamma_a^2 (s_a \cdot s_b) \left\{ (n_a \cdot n_b) I - n_b \otimes n_a \right\} \]
  • climb \[ N_{ab}^c = \gamma_a^2 (s_a \cdot s_b) n_a \otimes n_b \]

• core energy (slip plane)
\[
\psi_G(\nabla \phi) = \psi_{G0} \sum_{a,b} \nabla \phi_a \cdot N_{ab}^g \nabla \phi_b
\]

(Mianroodi & Svendsen, 2014)
atomistics-based PF energy scaling

- energy modeling
  - atomistics (molecular statics) exact, continuum (phase field) approx.
  - minimize error: atomistics-based continuum energy scaling

- scaled energy (density)
  \[
  \psi = \frac{\kappa_G g_0}{\kappa_H l_0} \left( f_E + f_H \right) + \frac{g_0 l_0}{\kappa_H \kappa_G} f_G
  \]

- energy, core size (molecular statics)
  \[
  g_0 = \int_{-\infty}^{\infty} \psi \, dx, \quad l_0 = \frac{\phi(+\infty) - \phi(-\infty)}{|\partial_x \phi(0)|}
  \]

- scaling factors (analytic)
  \[
  \kappa_H = \int_{\phi(-\infty)}^{\phi(+\infty)} \frac{f_{EH}(\phi) + \Delta f_{EH}(\phi)}{\sqrt{\Delta f_{EH}(\phi)}} \, d\phi, \quad \kappa_G = \frac{\phi(+\infty) - \phi(-\infty)}{\sqrt{\Delta f_{EH}(\phi(0))}}
  \]
  \[
  \Delta f_{EH}(\phi) = f_{EH}(\phi) - f_{EH}(0)
  \]

(Mianroodi & Svendsen, 2014)
disregistry match between PF and MS

- for dissociated screw in Cu
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modeling / numerical details

- 2 phase fields per \{111\} glide plane
  - 8 total for fcc single crystal
- MS-informed phase field
  - elasticity, SFE from MS
  - SFE: numerical look-up table
  - interface (homogeneous + gradient) energy scaling
    - interface energy (core energy, slip plane)
    - interface width (core size, slip plane)
- Green-function-based non-local elasticity (Eshelby, Mura, …)
- semi-implicit time integration (TDGL)
- spectral / FFT-based spatial methods

(Mianroodi & Svendsen, 2014)
dislocation dissociation

- initial straight ideal dislocation
  - energy minimization in MS with FIRE & CG
  - energy minimization in PF with GL

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<th>edge [Å]</th>
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* denotes core size.

(Mianroodi & Svendsen, 2014)
loading direction & energy pathways

- initial state ideal \((\phi_1, \phi_2) = (1, 0)\)
- \(E_{11}\) : ideal contraction \((0,0)\)
- \(E_{22}\) : ideal expansion \((1,0)\)
- \(E_{33}\) : partial expansion \((0.5,0.5)\)
- \(E_{33}\) : ideal expansion \((0.5,1.5)\)

\[(\bar{\phi}_1, \bar{\phi}_2) = (\bar{\phi}_1, \bar{\phi}_2) = (1, 0)\]

(Mianroodi & Svendsen, 2014)
E_{33} loading: comparison Cu & Al

increasing loading

Cu

Al

(Mianroodi & Svendsen, 2014)
multiple planes: slip in Al

• 1 initial (111) loop, uniaxial compression

(Mianroodi & Svendsen, 2014)
multiple planes: twinning in Cu

• 1 initial (111) loop, uniaxial compression

(Mianroodi & Svendsen, 2014)
level of SFE & glide or twinning

• “high” SFE (Al): almost ideal, tendency to glide
• “low” SFE (Cu): dissociated, tendency to twin
• agree with MD trends

(Mianroodi & Svendsen, 2014)
summary

• two approaches to dislocation line modeling: PN & PF

• elastic energy: PN & PF formulations equivalent for homogeneous elasticity
  • heterogeneous elasticity (bicrystal, twinning, etc.) only with PF

• gradient term (PF): correction to rigid approximation for SFE

• PF approach applied to dislocation based
  • dissociation
  • glide
  • twinning
Thank you for your attention!