Theory, Modeling and Simulation of the Collective Behavior of Dislocations

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(1) Introduction to dislocations and plasticity
(2) Simulation strategies
   - discrete dislocation dynamics in 2D and 3D
   - phase-field simulations
(3) Coarse-graining strategies
   - temporal
   - spatial
(4) Scaling and intermittency

A disclaimer: no quantum mechanics (today)!
Macroscopic deformation in fcc metals

![Graph showing stress-strain behavior]

- **I**: Elastic (slope $\sim \mu$)
- **II**: Slope $\sim \mu/10000$
- **III**: Slope $\sim \mu/200$

*single crystal under single slip*

$\mu$ is the shear modulus
Macroscopic deformation in $fcc$ metals

Mughrabi, Phil. Mag. 23, 869 (1971)

All micrographs from a Cu single crystal

Mughrabi, Phil. Mag. 23, 869 (1971)


dark lines in micrographs are dislocations

$\varepsilon^p = b \rho \langle x \rangle$

Single crystal under single slip

$\mu$ is the shear modulus

Mughrabi, Phil. Mag. 23, 869 (1971)
Macroscopic deformation in fcc metals

- only a few macrovariables are relevant
  suggestive of inherent spatial coarse graining

single crystal under single slip
μ is the shear modulus

ε_p = bρ⟨x⟩

Mughrabi, Phil. Mag. 23, 869 (1971)

# Multiscale landscape

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Each level is based on different methods and often done by different groups.

How do we link these together?
Dislocations are curvilinear topological defects that “carry” deformation.

Burgers vector ($\vec{b}$) measures displacement.

Edges defined by $\vec{b} \perp \hat{\xi}$. Note: dislocations are “signed.”

Concept connecting flow of dislocations to deformation dates to 1934.

- E. Orowan, Z. Physik, 84, 605 (1934)
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Other types of dislocations

screw dislocation has $\vec{b} \parallel \hat{\xi}$

In general, dislocations are of mixed character:

- dislocations cannot end in a crystal
  - must exist as loops or end at surfaces or other defects
- the Burgers vector is constant for each dislocation loop
- must obey crystallographic constraints

Screw dislocation structure and movement.

“Mixed” dislocation
Crystallographic constraints

Owing to constraints of edge components, most dislocation movement is planar.

Movement off plane is atomic-level activated process.

In 3D, dislocations on other slip planes act as barriers to dislocation motion:
Dislocations are not conserved

Frank-Read source:

Dislocations of opposite sense can annihilate each other:

Dislocation density increases with deformation:

\[ \rho_{\text{obs}} = \tau^2 \left( \alpha \mu b \right)^2 \]
Dislocations are not conserved

Frank-Read source:

Dislocations of opposite sense can annihilate each other:

Dislocation density increases with deformation:

\[ \rho_{\text{obs}} = \tau^2 \left( \frac{\alpha \mu b}{2} \right)^2 \]
Isotropic linear elasticity

Strain is derivative of displacement ($u$):

$$\varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) = \frac{1}{2} (u_{i,j} + u_{j,i}) \quad (f_{,i} = \frac{\partial f}{\partial x_i})$$

Relation between stress and strain:

$$\sigma_{kl} = c_{kli, j} \varepsilon_{ij}$$

$$c_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$$

We assume isotropic, linear elasticity:

• elastic properties independent of direction

$$\sigma_{11} = (\lambda + 2\mu) \varepsilon_{11} + \lambda \varepsilon_{22} + \lambda \varepsilon_{23}$$

$$\sigma_{12} = 2\mu \varepsilon_{12}$$

Elastic constants:

$$\mu = c_{44} \quad \lambda = c_{12} \quad \nu = \frac{\lambda}{2(\lambda + \mu)}$$

Have formalism for anisotropic elasticity.
Dislocation interactions are long ranged and anisotropic

Peach-Koehler force: \[
\frac{\vec{F}}{L} = (\vec{b} \cdot \vec{\sigma}) \times \hat{\xi} = \varepsilon_{ijk} b_l \sigma_{jl} \xi_k \hat{x}_i
\]

\[
\sigma_{ij} = \frac{\mu b_n}{8\pi} \oint_C \left[ R_{mp} (\varepsilon_{jmn} dl_i + \varepsilon_{imn} dl_j) \right] \frac{2}{1 - \nu} (R, i jm - \delta_{ij} R, ppm) \varepsilon_{kmn} dl_k
\]

Total stress (linear elasticity):

\[
\bar{\sigma}_i = \bar{\sigma}_{app} + \bar{\sigma}_i^{self} + \sum_{j \neq i} \bar{\sigma}_j
\]

Long-ranged interactions:

\[F \sim 1/R^2, \ E \sim 1/R\]
Energetics

Dislocation density tensor: continuous, discrete

Kosevich:

\[ E_I = \frac{\mu}{16\pi} \int \int \varepsilon_{ipl} \varepsilon_{jmn} R_{,mp}(\vec{r}, \vec{r}') \, d\vec{r} \, d\vec{r}' \]

\[ \times \left\{ \rho_{jl}(\vec{r}) \rho_{in}(\vec{r}') + \delta_{ij} \rho_{kl}(\vec{r}) \rho_{kn}(\vec{r}') + \frac{2\nu}{1-\nu} \rho_{il}(\vec{r}) \rho_{jn}(\vec{r}') \right\} \]

Nelson-Toner:

\[ E[\rho(\vec{q})] = \frac{1}{2} \int d^3q \, K_{ijkl}(\vec{q}) \rho_{ij}(\vec{q}) \rho_{kl}(-\vec{q}) \]

\[ K_{ijkl} = \frac{\mu}{q^2} \left[ Q_{ik} Q_{jl} + C_{il} C_{kj} + \frac{2\nu}{1-\nu} C_{ij} C_{kl} \right] \]

\[ Q_{ij} = \delta_{ij} - \frac{q_i q_j}{q^2} \quad C_{ij} = \varepsilon_{ijk} \frac{q_k}{q} \]

\[ R = |\vec{r} - \vec{r}'| \]

\[ R_{,mp} = \frac{\partial^2 R}{\partial x_m \partial x_p} \]
Dynamics

Dynamics are dissipative: \( m(v) \ddot{a} = \vec{F} - \gamma \vec{v} \)

If inertial effects are not important, assume over damped dynamics (i.e., \( a=0 \))
\[
\vec{v} = \frac{\vec{F}}{\gamma} = M\vec{F}
\]

Velocity-dependent mass:
\[
m_s(v) = \frac{W_0}{v^2} \left( -\gamma^{-1} + \gamma^{-3} \right)
\]
\[
\gamma = \left(1 - \frac{v^2}{C^2}\right)^{1/2}
\]
\[
W_o = \frac{\mu b^2}{4\pi} \ln \left( \frac{R}{r_o} \right)
\]
Simulation strategies

Microstructures on a scale of many microns
- 1 µm$^3$ of copper includes approximately $10^{11}$ atoms
- standard molecular dynamics methods can be used only for small numbers of dislocations

Mesoscale simulations:
- *dislocations are the entities of the simulations*
- atomic-level effects included as models

Dislocations around crack tip in shocked Cu. Example from Lomdahl, Holian, et al.
2D model

Parallel dislocations: “vector” lattice gas of charged particles in 2D.

\[
\frac{F_i}{L} = \tau_{\text{ext}} b_i + \sum_j \frac{F_{ij}}{L} b_i b_j
\]

\[
\frac{F_{ij}}{L} = \frac{\mu}{4\pi(1-\nu)} \frac{x_{ij}(x_{ij}^2 - y_{ij}^2)}{(x_{ij}^2 + y_{ij}^2)^2}
\]

Note: \( b \) can be +/-

- sign change in \( F \) at 45°
- \( F \sim 1/R \) (2D), \( E \sim \ln R \)

Constraints lead to frustration
Long-range interactions - the Fast Multipole Method in 2D

\[
\frac{F_i}{L} = \tau_{\text{ext}} b_i + \sum_j \frac{F_{ij}}{L} b_i b_j
\]

\[
\frac{F_{ij}}{L} = \frac{\mu}{4\pi(1 - \nu)} x_{ij} (x_{ij}^2 - y_{ij}^2)
\]

Greengard-Rohklin method applied to dislocations:

Stress for edge interactions:

\[
\phi_c(z) = \cos \theta \ln(z) \quad \phi_s(z) = \sin \theta \ln(z)
\]

\[
\phi_x(z) = x\phi_c(z) \quad \phi_y(z) = y\phi_s(z)
\]

\[
\sigma_{xx} = \frac{\mu b}{2\pi(1 - \nu)} \left( 2 \operatorname{Im}(\phi_c'(z)) - \operatorname{Re}(\phi_x''(z)) + \operatorname{Re}(\phi_y''(z)) \right)
\]

Wang and LeSar, Phil. Mag. 71, 151 (1995)

Perform all expansions on generating functions
Microstructure formation


correlation functions:
Representation of dislocations in 3D.

We represent dislocation loops with splines:‡

\[
\vec{r}_i = (1 - 3u^2 + 2u^3)\vec{P}_i + (3u^2 - 2u^3)\vec{P}_{i+1} + (u - 2u^2 + u^3)\vec{T}_i + (-u^2 + u^3)\vec{T}_{i+1}
\]

Node points are \(\vec{P}_i\) and tangent vectors at each node are \(\vec{T}_i\).

\(\vec{T}_i\) are completely determined by continuous curvature at nodes.

Most other groups employ straight dislocation segments
• Kubin and coworkers, LLNL

Ghoniem and Sun, Phys Rev B 60, 128 (1999)
Dislocation dynamics

\[ \frac{\vec{F}}{L} = (\vec{b} \cdot \vec{\sigma}) \times \hat{\xi} = \varepsilon_{ijk} b_l \sigma_{jl} \xi_k \hat{x}_i \]

\[ \sigma_{ij} = \frac{\mu b_n}{8\pi} \int_C \left[ R_{,mpp}(\varepsilon_{jmn} dl_i + \varepsilon_{imn} dl_j) \right. \\
\left. + \frac{2}{1-\nu} (R_{,ijm} - \delta_{ij} R_{,ppm}) \varepsilon_{kmn} dl_k \right] (R_{,ijk} = \partial^3 R / \partial x_i \partial x_j \partial x_k) \]

\[ \vec{\sigma}_i = \vec{\sigma}_{app} + \vec{\sigma}_i^{self} + \sum_{j \neq i} N_{\text{dis}} \vec{\sigma}_j \]

Numerical integration along lines gives force on the nodes.

Equation of motion for nodes:

\[ \vec{x}(t + \delta t) = \vec{v}(t) \delta t \]

\[ \vec{v} = \vec{F} / \gamma = M \vec{F} \]
Basic dislocation motion and interactions

Time sequences of configurations:
(a) F-R source;
(b) Annihilation;
(c) Dipole;
(d) Junction.
Parallel algorithm

distribution of dislocations is inhomogeneous
- dislocations span regions
- long-range forces through multipole expansion

Development of dislocation microstructure

\[ \rho = 10^7 / \text{cm}^2 \]

\[ \rho = 2 \times 10^8 / \text{cm}^2 \]

\[ \rho = 7.5 \times 10^8 / \text{cm}^2 \]

\[ \varepsilon_{ij} = \varepsilon_{ij}^e + \varepsilon_{ij}^p \]

\[ \sigma_{kl} = c_{kl \ell j} \varepsilon_{ij}^e \]

\[ = c_{kl \ell j} (\varepsilon_{ij} - \varepsilon_{ij}^p) \]

\[ \dot{\varepsilon}^p = -\frac{1}{2V} \sum_{i=1}^{N} \int_{l(i)} v^{(i)} [n^{(i)} \otimes b^{(i)} + b^{(i)} \otimes n^{(i)}] dl^{(i)} \]
Energy-based modeling of dislocations

• dislocation content as order parameter
• Ginsburg-Landau dynamics
• Khachaturyan and coworkers in 3D

2D model:
• fundamental quantity is the slip $\xi$
• dislocation content is given by gradient of the slip

$$\beta_{ij}^p = \xi(y) m_{js} \quad u_{i,j} = \beta_{ij}^e + \beta_{ij}^p \quad \rho_{hi} = -\varepsilon_{hl,j} \beta_{ji,l}$$

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

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

$$\frac{\partial \xi(x)}{\partial t} = \frac{\delta E[\xi(x)]}{\delta \xi(x)} + \tau - \eta(x, \xi(x))$$

Large-scale deformation

2D model of 3D behavior:
• stress-strain in good agreement with experiment
• variance shows peak at Stage II-III (agrees with Szekely et al.)

Once number of obstacles “saturates”
• Stage III behavior

Mimics removal of LC locks (obstacles) that pin cell walls to reach steady-state.

Simulations and experiment indicate structures are fractal

From 2D phase field, we find same fractal dimension as experiment

• implies self-similarity extends from our structures to full cellular structure.
• we measure “cell” sizes as areas with no dislocations, extending scaling to smaller scales

\[ n(A) = CA^{-D} \]

\[ D \]

\[ \tau[10^{-3}\mu] \]


Materials Science and Engineering
IOWA STATE UNIVERSITY
Direct simulations are computationally challenging

Time per force calculation \( t \sim L^2 \)
(length of dislocation), but \( L \propto \rho \propto \tau^2 \)

* time \( t \sim \tau^4 \)
* calculations slow down considerably as system is deformed
* too slow to include directly in continuum calculations
* we have formalism for O(N) simulation (FMM)
* some issues with boundary conditions

We are developing a coarse-graining approach that enables inclusion of dislocation content without resolving dislocation content.
Spatial coarse graining

Quest in coarse graining:
• identify a relatively small set of coarse-grained variables, selected from among a myriad of degrees of freedom
• describe system on larger length/time scales than practical (or possible) at scales associated with microscopic simulations

Coarse graining in other systems:
• systems exhibiting coupling on multiple scales, including turbulent fluids, critical magnets, mesoscale mechanics of solids, ...
• there has been some success for some systems

A critical question:
• Is the development of a CG for dislocations even possible?
Dislocation density tensor

Average dislocations over volume $\Omega$ to obtain the dislocation density tensor, $\rho_{ij}$

- first index is the line direction
- the second is the Burgers vector.

Limitations:

- $\rho_{ij}$ is an average
- no information about structure and energy within $\Omega$
- no information about crystallography
- no differentiation between stored and “geometrically necessary” dislocations
- unclear what sets optimal length scale for $\Omega$
- need evolution equations

\[ \rho_{\alpha\beta} = \sum_i b_\beta(i) \oint_{C_i} dl_\alpha(i) \]

Development of a density functional

\[
E_I = \frac{\mu}{16\pi} \int \int \varepsilon_{ipl} \varepsilon_{jmn} R_{,mp}(\vec{r}, \vec{r}') d\vec{r} d\vec{r}'
\]
\[
\times \left\{ \rho_{jl}(\vec{r}) \rho_{in}(\vec{r}') + \delta_{ij} \rho_{kl}(\vec{r}) \rho_{kn}(\vec{r}') + \frac{2\nu}{1 - \nu} \rho_{il}(\vec{r}) \rho_{jn}(\vec{r}') \right\}
\]

We divide space into regions with volume \( \Omega \).

Moment expansion of \( E_I \)

- find good convergence with gradient expansion (first order)
- does not provide information on structures smaller than \( \Omega \)

\[
R = |\vec{r} - \vec{r}'|
\]
\[
R_{,mp} = \frac{\partial^2 R}{\partial x_m \partial x_p}
\]

LeSar and Rickman, PRB (2004)
Multipole expansion of dislocation interactions.

Volume of point charges.

\[ \Phi(\vec{r}) = \sum_j \frac{q_j}{|\vec{r} - \vec{r}_j|} \approx \frac{Q}{R} + \frac{\vec{\mu} \cdot \vec{R}}{R^3} + \ldots \]

\[ Q = \sum_j q_j \]

\[ \vec{\mu} = \sum_j q_j \vec{r}_j \]

\[ \sigma_{ij} = \frac{\mu b_n}{8\pi} \oint \left[ R_{mpp} (\epsilon_{jmn} dl_i + \epsilon_{imn} dl_j) + \frac{2}{1-\nu} \epsilon_{kmn} (R_{i,jm} - \delta_{ij} R_{ppm}) dl_k \right] \]

\[ \rho_{\alpha\beta} = \sum_i b_\beta(i) \oint_{C_i} dl_\alpha(i) \]

\[ \rho_{\alpha\beta\gamma} = \sum_i b_\beta(i) \oint_{C_i} r_\gamma(i) dl_\alpha(i) \sim \nabla_\gamma \rho_{\alpha\beta} \]

LeSar and Rickman, PRB 65, 144110 (2002)

Volume of dislocation loops.
Multiple length scales

Polygonization:
• dislocations form walls
• structures within walls

Are there scaling laws that connect across scales?

What is the impact of substructure on mechanical properties?

We are developing local governing equations for substructure energetics and dynamics
• define coarse-graining length
Temporal coarse graining

Phenomenological approach (Holt, Rickman and Viñals):

\[
\frac{\partial}{\partial t} \rho_{ij} + \varepsilon_{ilm} \frac{\partial}{\partial x_l} j_{mj} = 0 \quad \text{conservation of Burgers vector}
\]

\[
\vec{j} \propto \nabla \frac{\delta E}{\delta \tilde{\rho}} \quad \text{flux law}
\]

Connection to mesoscale simulation:

\[
\left\langle \rho_{ij}(\vec{q},t) \rho_{mn}(-\vec{q},t) \right\rangle \quad \text{dynamical structure factor}
\]

\[
S_{\text{loop}} \propto \iint \int dsds' \left\langle \exp \left[ i\vec{q} \cdot \left( \tilde{R}(s,t) - \tilde{R}(s',t') \right) \right]\right\rangle \quad \text{polymer loop structure factor}
\]
Finite temperature effects

Thermally-induced kinks and jogs lead to entropic interactions between dislocations.

- analogues:
  - dipolar chains in electrorheological fluids
  - Type II superconductors (Halsey and Toor)

Energetics (Kosevich, Nelson-Toner):

\[
E[\rho(\tilde{q})] = \frac{1}{2} \int d^3q K_{ijkl}(\tilde{q})\rho_{ij}(\tilde{q})\rho_{kl}(\tilde{-q})
\]

\[
K_{ijkl} = \frac{\mu}{q^2} \left[ Q_{ik}Q_{jl} + C_{il}C_{kj} + \frac{2\nu}{1-\nu} C_{ij}C_{kl} \right]
\]

\[
Q_{ij} = \delta_{ij} - \frac{q_iq_j}{q^2} \quad C_{ij} = \varepsilon_{ijk} \frac{q_k}{q}
\]

Rickman and LeSar, PRB 64, 94106 (2001)
Isolated line defects: theory of distributions

- e.g., straight screw along $z$

$$\rho_{ij}(\vec{r}) = b \delta_{i3} \delta_{j3} \delta(x) \delta(y)$$

- energy between straight dislocations

$$e_{\text{straight}}(a) = -\frac{\mu b^{(1)} b^{(2)}}{2\pi} \ln(a)$$

$$\int d^2q \frac{1}{q^2} \exp(-iq_a) = -2\pi \ln(a)$$

Thermally induced kinks and jogs:

- Fourier expansion in modes
Temperature-dependent force

\[ \int d^2q \frac{1}{q^2 + k^2} \exp(-iq \cdot a) = 2\pi K_0(ka) \]

partition function

\[ Z = N \left[ \int d\omega_\perp \exp\left(\frac{-L_\Delta e_\perp}{kT}\right) \right] \left[ \int d\omega_\perp \exp\left(\frac{-L_\Delta e_\perp}{kT}\right) \right] \]

free energy

\[ F = -kT \ln(Z) \]

force

\[ f = -\frac{\partial F}{\partial a} \]

kT \ll elastic force
Temperature and noise

\( kT << \) elastic energies
  - effect of thermal noise mainly through atomic-level processes (cross slip, climb, jogs)

Noise arises from fluctuations in long range strain fields
  - multiplicative

Some work has been done with simple rate equations with added multiplicative noise term:
  - Hahner et al: fractal structures
  - our group: wall stability
Thermodynamics of local order

Find that ordering, noise, energetics all functions of dislocation density - define force for ordering

noise: \( R \sim \rho^{1/2} \)

structural order: \( \alpha = -0.36 \pm 0.01 \)
\( \xi_w \propto R^{-0.73} \)

energy: \( E_{\text{int}} \propto -\rho^{\alpha} \)
\( \alpha = 0.998 \pm 0.001 \)

force: \( \xi_w(t,N) = - \left. \frac{\partial E}{\partial t} \right|_N \frac{\partial \xi_w}{\partial t} \)
\( \xi_w(2\tau) \propto \rho^{\beta} \)
\( \beta = 0.94 \pm 0.05 \)

C(x,y) = standard correlation function

\( q(x) = \sum_y C(x,y) \)
\( \xi_w = \sum_{q(x)>q_{\text{random}}} q(x) \)

Data provides measure of intermittent flow

**Pond, 1972**

![Graph showing resolved shear as a function of time for 19 slip bands](image)

*Fig. 6. Resolved shear for each slip band as a function of time for 19 slip bands is shown for an aluminum single crystal extended at 100 °C.*

**Acoustic emission experiments:**

![AE signal graph](image)

Find power law distribution of avalanche size with exponent 1.6 - 2.0.  
*Vinogradov et al., Phil Mag A 81, 1427 (2001)*

**Ice crystal**

![Power law distribution graph](image)

*\( \tau_E = 1.6 \)

*Miguel et al., Nature, 2001*
Phase-field simulations

Employed phase-field calculations as before:
• in Stage I
• stress raised in small increments

Bursts during one loading step:

\[ N(A) = CA^{-\sigma} \]
\[ \sigma \approx 1.8 \pm 0.1 \]

Phase-field simulations show avalanche behavior:
• power-law scaling
• same class as fracture, earthquakes, ...
• example of self-organized critical system?

M. Koslowski, R. LeSar, and R. Thomson,
Small-scale deformation

Uchic, Dimiduk et al. in Science and Acta Mater.
Direct measurement of intermittent behavior in deformation

\[ N(d) \propto d^{-\sigma} \]

\[ \sigma \sim 1.60 \pm 0.01 \]

Implications

Simulations and experiment indicate that dislocations form self-organized critical systems.

Enables us to employ a new set of theories and analysis in dislocation theory.
Other recent theoretical work of note

Javier Gil Sevillano - size effects (with analogy to flow through porous media)

Michael Zaiser - scaling, statistical mechanics of dislocations

Anter El Azab - kinetic theory of dislocations

Jim Sethna - mesoscale theory based on continuous dislocation theory

Ishtvan Groma - Debye screening in dislocations

...
How far have we progressed as a field?

A. H. Cottrell:

In 1953 said of strain hardening that "it was the first problem to be attempted by dislocation theory and may be the last that is solved"

In 2002, Cottrell summed up progress since 1953 by stating that "It is sometimes said that the turbulent flow of fluids is the most difficult remaining problem in classical physics. Not so. Work hardening is worse"

After 50 years, still much to understand about the relation of dislocation structure and mechanical response.
QUESTIONS?