Microstructure Mechanics
Dislocation dynamics

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Dislocations and strain hardening

\[ \frac{d\sigma}{d\varepsilon} \]

\( \sigma \)

\( \varepsilon \) true strain

\( \sigma \) stress

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Dynamics: forces among dislocations

Dislocation 2 “feels” the stress field of dislocation 1 (and vice versa).

Peach-Koehler Force

\[ \vec{F}_{1\rightarrow2} = \left( \sigma^{1\rightarrow2} \vec{b}_2 \right) \times \vec{t}_2 \]

- \( \sigma_{xy} \) – produces glide force
- \( \sigma_{xx} \) – produces climb force
Forces among edge dislocations

\[ F_{\text{glide}} = \frac{Gb^2}{2\pi(1-v)} \frac{\Delta x(\Delta x^2 - \Delta y^2)}{(\Delta x^2 + \Delta y^2)^2} \]

\[ \sigma_{xx} = -D y \frac{3\Delta x^2 + \Delta y^2}{(\Delta x^2 + \Delta y^2)^2}, \quad \text{with:} \quad D = \frac{Gb}{2\pi(1-v)} \]

\[ \sigma_{xy} = \sigma_{yx} = D \Delta x \frac{\Delta x^2 - \Delta y^2}{(\Delta x^2 + \Delta y^2)^2} \]
Forces among edge dislocations

\[ \sigma_{xx} = -D \frac{3 \Delta x^2 + \Delta y^2}{(\Delta x^2 + \Delta y^2)^2}, \quad \text{with}: \quad D = \frac{Gb}{2\pi(1-v)} \]

\[ \sigma_{xy} = \sigma_{yx} = D \Delta x \frac{\Delta x^2 - \Delta y^2}{(\Delta x^2 + \Delta y^2)^2} \]
Forces among screw dislocations

Dislocation 2 “feels” the stress field of dislocation 1 (and vice versa).

\[ \sigma_{\theta z} = \sigma_{z \theta} = \frac{Gb}{2\pi r} \]

So force on dislocation 2 from dislocation 1 is:

\[ F = \frac{Gb^2}{2\pi r} \]

... but this force acts in the radial direction.

Force on dislocation 2 from dislocation 1, resolved onto the glide plane is:

\[ F_{\text{res}} = \frac{Gb^2}{2\pi r} \cos \theta \]

Alternatively, we can use the stress field expressed in Cartesian co-ordinates:

\[ \sigma_{xx} = \sigma_{yy} = \sigma_{zz} = \sigma_{xy} = \sigma_{yx} = 0 \]

\[ \sigma_{xz} = -\frac{Gb}{2\pi} \frac{\Delta y}{\Delta x^2 + \Delta y^2} = -\frac{Gb \sin \theta}{2\pi r} \]

\[ \sigma_{yz} = \frac{Gb}{2\pi} \frac{\Delta x}{\Delta x^2 + \Delta y^2} = \frac{Gb \cos \theta}{2\pi r} \]

Note that the shear stress acting to shear atoms parallel to \( \mathbf{b} \) above and below the glide plane is \( \sigma_{yz} \).

\[ F_{\text{res}} = \sigma_{yz} \mathbf{b} = \frac{Gb^2}{2\pi r} \cos \theta = \frac{Gb^2}{2\pi} \frac{\Delta x}{\Delta x^2 + \Delta y^2} \]
Stable configurations for dislocation ensembles

For **like** Burgers vectors:
- $\Delta x = \pm \Delta y$: unstable equilibrium
- $\Delta x = 0$: stable equilibrium

For **opposite** Burgers vectors:
- $\Delta x = \pm \Delta y$: stable equilibrium
- $\Delta x = 0$: unstable equilibrium

For a set of "**opposite**" Burgers vectors:

There are a large number of possible stable arrangements.

These stable arrangements have minimal long-range stress fields.

For **like** Burgers vectors:
- Stable array is a planar stack
- A low angle tilt boundary.
- This arrangement has a strong long-range stress field.

"Taylor lattice"

"Dipole dispersion"
Calculate the mutual forces for the following dislocation configurations:

2 parallel edge dislocations (same glide plane)
parallel edge and screw dislocations (same glide plane)
2 parallel screw dislocations (same glide plane)
2 parallel edge dislocations (above each other)
2 anti-parallel edge dislocations (same glide plane)

Write program:
store: stress fields of 2D infinite screw and edge dislocations (along z axis)
enter: position (x,y) and Burgers vector b of second dislocation (place first dislocation in origing)
Discrete Dislocation Dynamics
Statistical Dislocation Dynamics
Discrete Dislocation Dynamics
Discrete Dislocation Dynamics in 2D

2D – view parallel to dislocation line
Discrete Dislocation Dynamics in 2D

2D – view parallel to dislocation line

Some questions:
Difference between edge and screw dislocations?
How to do multiplication?
Dislocation bow-out?
Annihilation?
Climbing?
Discrete Dislocation Dynamics in 2D

2D – view into the glide plane
Discrete Dislocation Dynamics in 2D

2D – view into the glide plane

Some questions:
Difference between edge and screw dislocations?
Cross-slip?
Cutting?
Jog-drag?
3D: DDD (discrete dislocation dynamics)
Discrete Dislocation Dynamics in 3D

Full 3D segment treatment

Some questions:
Difference between edge and screw dislocations?
Junctions?
Cutting?
Cores of the dislocations?
Discrete Dislocation Dynamics in 2D

2D – view parallel to dislocation line

Principle procedure
How to proceed?

Stress field of (edge) dislocation
Get coordinates
Use Peach Koehler
Move it
Force on dislocation ‘a’
by all others

\[ \vec{F}_a = \left( \sigma_{\text{all others} \rightarrow a} \vec{b}_a \right) \times \vec{t}_a \]
Basics of Discrete Dislocation Dynamics in 2D

Force

\[ \vec{F}_a = \left( \sigma \mathrel{\underbrace{\text{all others} \rightarrow a}} \vec{b}_a \right) \times \vec{t}_a \]

Motion

\[ \vec{F} = m \ddot{x} + B\dot{x} \approx B\dot{x} \]

- acceleration
- friction coefficient (drag)
- inertia
- velocity
Equilibrium of forces

\[ \sum \vec{F}_i = 0 \]

\[ \sum \vec{F}_i = B\ddot{x} + \vec{F}_a = 0 \]

\[ \vec{F}_a = \left( \sigma^{\text{alle} \rightarrow a} \vec{b}_a \right) \times \vec{t}_a \]
Equilibrium of forces

\[ \sum F = 0 \]

\[ F_{\text{disloc}} + F_{\text{self force}} + F_{\text{extern}} + F_{\text{therm}} + F_{\text{viscous}} + F_{\text{obstacle}} + F_{\text{Peierls}} + F_{\text{osmotic}} + F_{\text{image}} + F_{\text{inertia}} \]

- \( F_{\text{disloc}} \): elastic – other dislocations
- \( F_{\text{self force}} \): elastic – self
- \( F_{\text{extern}} \): external
- \( F_{\text{therm}} \): Stochastic Langevin
- \( F_{\text{viscous}} \): viscous drag
- \( F_{\text{obstacle}} \): obstacle
- \( F_{\text{Peierls}} \): Peierls
- \( F_{\text{osmotic}} \): chemical forces
- \( F_{\text{image}} \): surface forces
Example of Discrete Dislocation Dynamics in 2D

\[ \sigma_{xz} = \sigma_{zx} = \sigma_{yz} = \sigma_{zy} = 0 \]

\[ \sigma_{xx} = -Dy \frac{3x^2 + y^2}{(x^2 + y^2)^2}, \quad \text{with:} \quad D = \frac{Gb}{2\pi(1 - \nu)} \]

\[ \sigma_{yy} = Dy \frac{x^2 - y^2}{(x^2 + y^2)^2} \]

\[ \sigma_{xy} = \sigma_{yx} = Dx \frac{x^2 - y^2}{(x^2 + y^2)^2} \]

\[ \sigma_{zz} = v(\sigma_{xx} + \sigma_{yy}) \]

\[
\bar{F}_a = \left( \underbrace{\sigma_{all\rightarrow a}}_{\sigma} \bar{b}_a \right) \times \bar{t}_a
\]

\[
\bar{F}_a + B\ddot{x} + \bar{F}_{external} = 0
\]
Example of Discrete Dislocation Dynamics in 2D
1) Calculate stress field of machine and of all other dislocations at position of T

2) Use Peach-Koehler equation to get force on dislocation

3) Integrate with very small time step (explicit) viscous eq. of motion
3D segments and node construction

Burgers vector sum rule

- For each node
  \[ b_{01} + b_{02} + b_{03} = 0 \]
- For each segment
  \[ b_{01} + b_{10} = 0 \]
Set-up of Discrete Dislocation Dynamics in 3D

Annihilation events

Figure: Annihilation of two attractive dislocations
Jog formation

Figure: Jogs are formed when the angle between two attractive dislocations in different planes becomes less than a critical angle $\theta_c^{\text{jog}}$. 
Examples in 2D and 3D

Examples
Example of Discrete Dislocation Dynamics in 2D
Example of Discrete Dislocation Dynamics in 2D
Example of Discrete Dislocation Dynamics in 3D
Example of Discrete Dislocation Dynamics in 3D
Example of Discrete Dislocation Dynamics in 3D
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Example of Discrete Dislocation Dynamics in 3D
Example of Discrete Dislocation Dynamics in 3D
Example of Discrete Dislocation Dynamics in 3D
Example of Discrete Dislocation Dynamics in 3D
Example of Discrete Dislocation Dynamics in 3D: superalloys
Example of Discrete Dislocation Dynamics in 3D: superalloys
courtesy: Pratt and Whitney
Example of Discrete Dislocation Dynamics in 3D: superalloys
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WHY Statistical Dislocation Dynamics ?
• kinetic equation of state
• structure evolution
• coupling to continuum kinematics
Statistical Dislocation Dynamics

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Note: The diagram shows a grid with some symbols and annotations. The circled sections and annotations are not clearly legible in the image.
\[ \tau = G\gamma = \frac{Gb}{2\pi r} \]

\[ \rho = \frac{1}{a^2} \]

\[ \tau = \frac{Gb}{2\pi a} = \frac{Gb}{2\pi} \sqrt{\rho} \]
• kinetic equation of state

\[ \tau = \alpha G b \sqrt{\rho} \]
**kinetics**: collective dislocation behaviour

- kinetic equation of state

\[
\frac{d\rho}{d\gamma} = A\rho^+ + B\rho^-
\]

- structure evolution

\[
\dot{\gamma} = \frac{d\gamma}{dt} = n \frac{dx}{X} \frac{b}{Z} \frac{1}{dt} = \rho_m b v
\]