Hierarchy of dislocation mechanics

- one dislocation
- parallel loops (Kubin)
- reactions (Kubin)
- mesoscopic boundary conditions (grain / orientation neighborhood)
- spin (orientation change)
Dislocation character

- **Screw dislocation**
- **Slip plane**
- **Edge dislocation line**
- **Extra row of atoms**
Kinematics, displacement

\[ u = u(x, y, z) \]

\[ u(x_1, y, z) = u_1(x, y, z) \]
\[ u(x_2, y, z) = u_2(x, y, z) \]

\[ u(x_1, y, z) = u_1(x, y, z) \]
\[ u(x_2, y, z) = u_2(x, y, z) \]
Kinematics, displacement

\[ u = u(x, y, z) \]

\[ u(1)(x, y, z) \neq u(2)(x, y, z) \]
Displacement vector:
\[ \mathbf{u} = [u_x, u_y, u_z] \]

Strain tensor:
\[ \varepsilon_{xx} = \frac{\partial u_x}{\partial x} \]
\[ \varepsilon_{xy} = \frac{1}{2} \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) \text{ etc.} \]

Dilatation, \( \Delta \):
\[ \Delta = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} \]
Strain field of straight screw dislocation

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

\[
\varepsilon_{xz} = \frac{1}{2} \frac{\partial u_z}{\partial x} = \frac{b}{4\pi} \frac{\partial}{\partial x} \tan^{-1}\left(\frac{y}{x}\right)
\]

\[
= -\frac{b}{4\pi} \frac{1}{1 + \left(\frac{y}{x}\right)^2} \frac{y}{x^2}
\]

\[
= -\frac{b}{4\pi} \frac{y}{x^2 + y^2} = -\frac{b}{4\pi} \frac{\sin \theta}{r}
\]

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\varepsilon_{yz} = \frac{1}{2} \frac{\partial u_z}{\partial y} = \frac{b}{4\pi} \frac{\partial}{\partial y} \tan^{-1}\left(\frac{y}{x}\right)
\]

\[
= \frac{b}{4\pi} \frac{1}{1 + \left(\frac{y}{x}\right)^2} \frac{1}{x}
\]

\[
= \frac{b}{4\pi} \frac{x}{x^2 + y^2} = \frac{b}{4\pi} \frac{\cos \theta}{r}
\]

"Recipe":
- take a hollow cylinder, axis along z;
- cut on a plane parallel to the z-axis;
- displace the free surfaces by \(b\) in the z-direction.

By inspection:
\[
u_x = u_y = 0
\]

\[
u_z = \frac{b\theta}{2\pi}
\]

\[
= \frac{b}{2\pi} \tan^{-1}\left(\frac{y}{x}\right)
\]
Displacement and stress field

**Stress field of straight screw dislocation**

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

\[
\varepsilon_{xz} = -\frac{b}{4\pi} \frac{y}{x^2 + y^2} = -\frac{b}{4\pi} \frac{\sin\theta}{r}
\]

\[
\varepsilon_{yz} = \frac{b}{4\pi} \frac{x}{x^2 + y^2} = \frac{b}{4\pi} \frac{\cos\theta}{r}
\]

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

\[\Delta = 0\]

\[
\sigma_{xz} = 2G\varepsilon_{xz} = -\frac{Gb}{2\pi} \frac{y}{x^2 + y^2} = -\frac{Gb \sin\theta}{2\pi} \frac{1}{r}
\]

\[
\sigma_{yz} = 2G\varepsilon_{yz} = \frac{Gb}{2\pi} \frac{x}{x^2 + y^2} = \frac{Gb \cos\theta}{2\pi} \frac{1}{r}
\]

In Polar coordinates:

(either by direct inspection, or by transforming the strains and stresses from Cartesian co-ordinates)

\[
\varepsilon_{\theta z} = \varepsilon_{z\theta} = \frac{b}{4\pi r}
\]

All other components of the stress tensor are zero.

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

Note:
- Stress and strain fields are pure shear
- Fields have radial symmetry
- Stresses and strains are proportional to \(1/r\):
  - extend to infinity
  - tend to infinite values as \(r \to 0\)

Infinite stresses cannot exist in real materials: the dislocation core radius \(r_0\) is that within which our assumption of linear elastic behaviour breaks down. Typically \(r_0 \approx 1\) nm.
Forces between edge dislocations

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

The important components of the stress field are:

\[ \sigma_{xy} \] produces glide force on disln 2;

\[ \sigma_{xx} \] produces climb force on disln 2.

\[ \sigma_{xx} = -D \frac{3 \Delta x^2 + \Delta y^2}{(\Delta x^2 + \Delta y^2)^2} \]

with:

\[ D = \frac{Gb}{2\pi(1-\nu)} \]

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

So glide force, resolved onto the slip plane, is:

\[ F_{\text{glide}} = \frac{Gb^2}{2\pi(1-\nu)} \frac{\Delta x (\Delta x^2 - \Delta y^2)}{(\Delta x^2 + \Delta y^2)^2} \]
Forces between 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 \( b \) above and below the glide plane is \( \sigma_{yz} \):

\[ F_{\text{res}} = \sigma_{yz} b = \frac{Gb^2}{2\pi r} \cos \theta = \frac{Gb^2}{2\pi} \frac{\Delta x}{\Delta x^2 + \Delta y^2} \]
Stable arrangements for edge dislocations

For \textbf{like} Burgers vectors:
\[ \Delta x = \pm \Delta y: \text{unstable equilibrium} \]
\[ \Delta x = 0: \text{stable equilibrium} \]

For \textbf{opposite} Burgers vectors:
\[ \Delta x = \pm \Delta y: \text{stable equilibrium} \]
\[ \Delta x = 0: \text{unstable equilibrium} \]

For a set of “\textbf{opposite}” Burgers vectors:

There are a large number of possible stable arrangements.

For \textbf{like} Burgers vectors:
Stable array is a planar stack

A low angle tilt boundary.

This arrangement has a strong long-range stress field.

“These stable arrangements have minimal long-range stress fields.”
Forces on dislocations

Dislocation motion only has "meaning" normal to the line vector.

Forces on dislocations can only act normal to the line vector.
Strain rate from motion of dislocations

If a dislocation moved the whole length of the crystal $d$, it would contribute $b$ to the displacement $D$.

If each dislocation moves an amount $x_i$ (less than $d$), then each will contribute $(x_i / d) \cdot b$ to $D$.

$$D = \frac{b}{d} \sum x_i$$

Shear strain is:

$$\varepsilon = \frac{D}{h} = \frac{b}{dh} \sum x_i$$

Define average distance moved by each dislocation:

$$\bar{x} = \frac{1}{N} \sum x_i$$

Density of mobile dislocations is:

$$\rho_m = \frac{N}{hd}$$

Strain rate:

$$\dot{\varepsilon} = \frac{d\varepsilon}{dt} = b\rho_m \frac{d\bar{x}}{dt} = b\rho_m \bar{v}$$

- where $\bar{v}$ is the average dislocation glide velocity.
Real dislocations
Real dislocations
Real dislocations
Real dislocations
Real dislocations
Real dislocations
Real dislocations
Real dislocations