Energy of Dislocations

Plastic Deformation in Crystalline Materials

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Lecture 7

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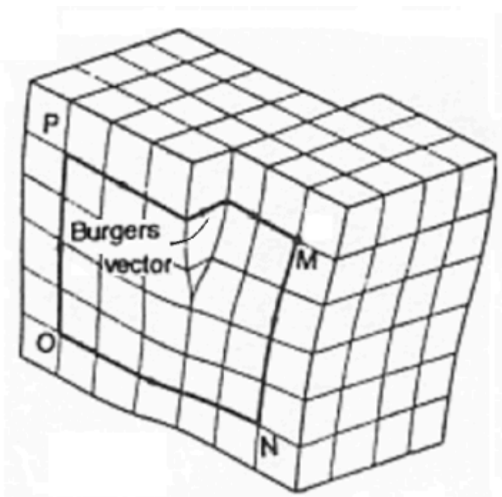
Elastic Fields around Screw Dislocation



$$u_z = \frac{b}{2\pi}\theta = \frac{b}{2\pi}\left\{\tan^{-1}\left(\frac{y}{x}\right) + \frac{\pi}{2}\mathrm{sgn}(y)\left[1 - \mathrm{sgn}(x)\right]\right\}$$

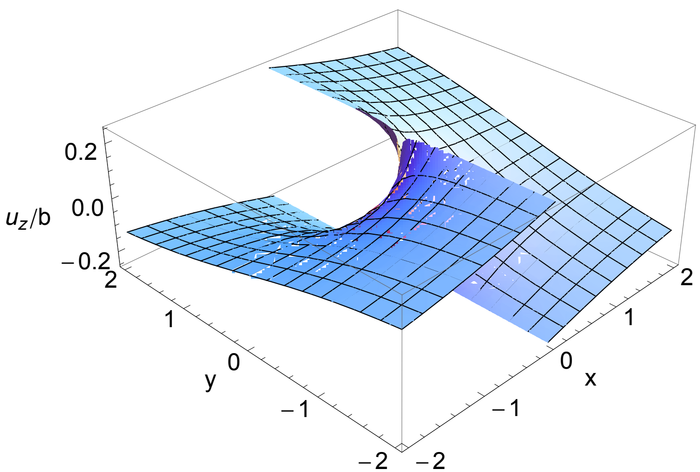
$$E_{rr} = \frac{\partial u_r}{\partial r} \qquad E_{\theta\theta} = \frac{1}{r}\frac{\partial u_\theta}{\partial \theta} + \frac{u_r}{r} \qquad E_{zz} = \frac{\partial u_z}{\partial z}$$

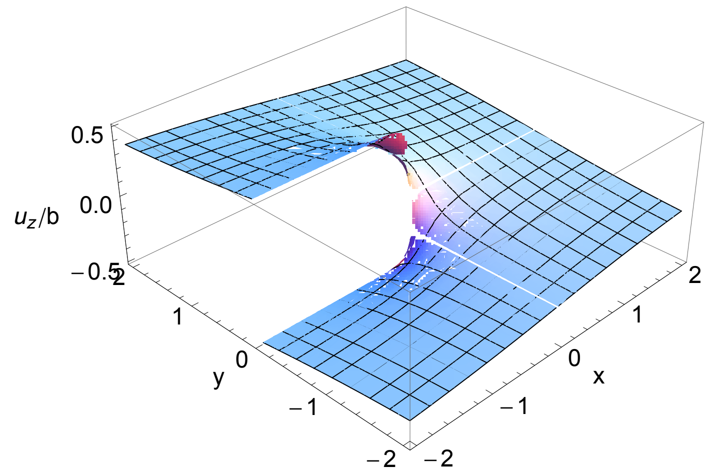
$$E_{r\theta} = \frac{1}{2}\left[\frac{1}{r}\frac{\partial u_r}{\partial \theta} + \frac{\partial u_\theta}{\partial r} - \frac{u_\theta}{r}\right] \qquad E_{\theta z} = \frac{1}{2}\left(\frac{\partial u_\theta}{\partial z} + \frac{1}{r}\frac{\partial u_z}{\partial \theta}\right)$$

$$E_{zr} = \frac{1}{2}\left(\frac{\partial u_z}{\partial r} + \frac{\partial u_r}{\partial z}\right),$$

$$\varepsilon_{z\theta} = \frac{b}{4\pi r} \quad \Rightarrow \quad \varepsilon_{xz} = -\frac{b}{4\pi}\frac{y}{r^2}, \qquad \varepsilon_{xy} = \frac{b}{4\pi}\frac{x}{r^2}$$

Importance of Additional Terms





$$u_z = \frac{b}{2\pi}\tan^{-1}\left(\frac{y}{x}\right)$$

$$u_z = \frac{b}{2\pi}\left\{\tan^{-1}\left(\frac{y}{x}\right) + \frac{\pi}{2}\,\mathrm{sgn}(y)\left[1-\mathrm{sgn}(x)\right]\right\}$$

$$\partial_x \tan^{-1}\left(\frac{y}{x}\right) = -\frac{y}{r^2} + \pi\,\mathrm{sgn}(y)\,\delta(x),$$

$$\partial_y \tan^{-1}\left(\frac{y}{x}\right) = \frac{x}{r^2}$$

$$\partial_y \mathrm{sgn}(y) = 2\,\delta(x).$$

$$\varepsilon_{zx} = \varepsilon_{zx}^{(e)} + \varepsilon_{zx}^{(p)} = \frac{1}{2}\partial_x u_z = \frac{b}{4\pi}\frac{-y}{r^2}$$

$$\varepsilon_{zy} = \varepsilon_{zy}^{(e)} + \varepsilon_{zy}^{(p)} = \frac{1}{2}\partial_y u_z = \frac{b}{4\pi}\left[\frac{x}{r^2} + 2\pi H(-x)\delta(y)\right]$$

Volterra Dislocations

Although the concept of dislocations was postulated in 1934 by Orowan, Polyani and Taylor, the stress field around them was calculated about 25 years before that by Volterra.

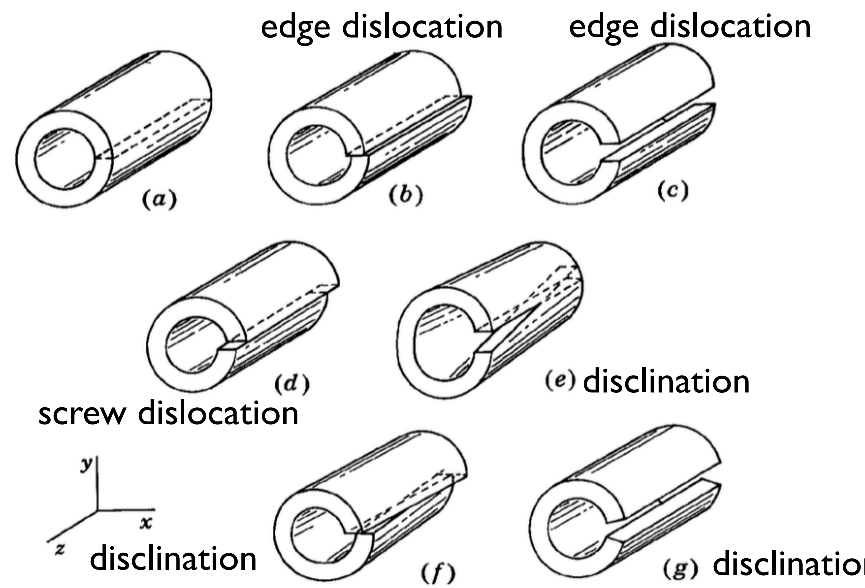


FIGURE 1-1. A cylinder (a) as originally cut, and (b) to (g), as deformed to produce the six types of dislocations as proposed by Volterra.

[Hirth & Lothe, Theory of Dislocations, Wiley, 1982]

Elastic Field around an Edge Dislocation

From theory of elasticity, we can calculate the elastic field of a Volterra's edge dislocation (see Timoshenko and Goodier).

Airy stress function

$$\chi = -\frac{\mu}{1-\nu}\frac{b}{2\pi} y \ln r$$

Displacement field

$$u_x = \frac{b}{2\pi}\left[\theta + \frac{1}{2(1-\nu)}\frac{xy}{r^2}\right],$$

$$u_y = -\frac{b}{8\pi(1-\nu)}\left[(1-2\nu)\ln r^2 + \frac{x^2-y^2}{r^2}\right],$$

Stress field

$$\sigma_{xx} = -\frac{\mu b}{2\pi(1-\nu)} y \frac{3x^2+y^2}{r^4},$$

$$\sigma_{yy} = \frac{\mu b}{2\pi(1-\nu)} y \frac{x^2-y^2}{r^4},$$

$$\sigma_{xy} = \frac{\mu b}{2\pi(1-\nu)} x \frac{x^2-y^2}{r^4},$$

$$\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$$

Elastic Field around an Edge Dislocation

- Another way to calculate the displacement field is:
  We know:

$$\varepsilon_{xy}^{p} = \frac{1}{2} b\ \delta(y) H(-x)$$

Then using micromechanics to calculate the displacement field.

- There are a couple of different ways to calculate the elastic field around an edge dislocation.

For example, Eshelby (1966):

$$u = \frac{b}{2\pi}\left(\tan^{-1}\frac{y}{x} + \frac{1}{2(1-\sigma)}\frac{xy}{r^2}\right)$$

$$v = \frac{b}{2\pi}\left(\frac{1-2\sigma}{2(1-\sigma)}\ln\frac{1}{r} + \frac{1}{2(1-\sigma)}\frac{y^2}{r^2}\right)$$

(In the above equations, *u* is u_x and *v* is u_y; σ is Poisson's ratio, ν)
while:

$$u_x = \frac{b}{2\pi}\left[\theta + \frac{1}{2(1-\nu)}\frac{xy}{r^2}\right],$$

$$u_y = -\frac{b}{8\pi(1-\nu)}\left[(1-2\nu)\ln r^2 + \frac{x^2-y^2}{r^2}\right],$$

Question: Why the formulae for u_y are different?

Remarks

- We assumed that dislocations are straight and stationary.
- We will learn how to calculate the elastic field around:
  - a curved dislocation
  - a moving dislocation
- We also assumed that the medium is isotropic!

Remarks - II

- Stress is proportional to μ and *b*

- All components of stress and strain fields are singular at *r* = 0 (in fact they are ~ 1/*r*). Not physical
  In other words, continuum theory breaks down in the vicinity of the dislocation line.

- For edge dislocation:
  $$u_x(x,0^+) - u_x(x,0^-) = b \text{ for } x<0$$
- For screw dislocation:
  $$u_z(x,0^+) - u_z(x,0^-) = b \text{ for } x<0$$

- As *r* goes to infinity, u_y also goes to infinity.
- The stress field of a screw dislocation contains only shear components, but the stress field of an edge has both shear and normal components.

Energy of Dislocations

- A crystal containing a dislocation is not in its lowest energy. The dislocation distorts the atoms around itself. This extra energy resulting from crystal distortion is the *strain energy*.

- The strain energy can be decomposed it into the elastic part E_{elastic} and the energy inside the nonlinear core E_{core}.

- The elastic (strain) energy density is equal to

$$\frac{1}{2}\sigma_{ij}\varepsilon_{ij}$$

Elastic Energy of a Screw Dislocation

Consider a hollow cylinder of inner radius r_0 and outer radius R and of length L. Let's put a screw dislocation at the center of the cylinder. The elastic energy due to the existence of the dislocation is:

$$E_{el} = \frac{1}{2}\int_V (\sigma_{z\theta}\varepsilon_{z\theta} + \sigma_{\theta z}\varepsilon_{\theta z})\,\mathrm{d}V = \int_V \sigma_{z\theta}\varepsilon_{z\theta}\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}z = \frac{L\mu b^2}{4\pi}\ln\left(\frac{R}{r_0}\right)$$

Elastic Energy of a Dislocation

- the elastic energy *per unit length* of the dislocation reads

$$E_{\mathrm{el}} = \frac{1}{2}\int_{r_0}^{R}\int_0^{2\pi} \sigma_{ij}\varepsilon_{ij}\, r\, \mathrm{d}\theta \mathrm{d}r = \frac{\mu b^2}{4\pi\kappa}\ln\left(\frac{R}{r_0}\right),$$

where

for screw: $\kappa = 1$
for edge: $\kappa = 1 - \nu$

- To avoid the core area where stress and strain fields diverge and elasticity breaks down, an inner cut-off radius $r = r_0$ is adopted. (usually $r_0 \sim b$)
- Here R is the outside radius of the crystal.

Elastic Energy of Mixed Dislocations

- The elastic energy of a mixed dislocation can be simply obtained by the superposition of the energies of its screw and edge parts

$$E_{\rm el} = \frac{\mu}{4\pi}\left[\frac{b^2\sin^2\theta}{(1-\nu)} + b^2\cos^2\theta\right]\ln\left(\frac{R}{r_0}\right),$$

θ = angle between $\vec{b}$ and line direction $\hat{\xi}$.

Remark – I

$$E_{\mathrm{el}} = \frac{\mu b^2}{4\pi\kappa} \ln\left(\frac{R}{r_0}\right)$$

- It is clear that $E_{el} \rightarrow \infty$ as $R \rightarrow \infty$.
- This means that the energy of a single dislocation inside an infinite medium diverges, which is an indication of the long range nature of the dislocation stress field.
- In reality, crystals contain many dislocations. These dislocations are apt to form in configurations in which the effects of the stress field extends only to the neighboring dislocation of opposite sign.
- In a random distribution of dislocations, this distance is approximately half the average spacing or $1/\rho^{0.5}$, where ρ is the density of dislocations
- Exercise: prove the average spacing is $1/\rho^{0.5}$.
- Exercise: Show that for a dislocation dipole made up of two opposite edge dislocations, the elastic energy is given by

$$E_{\mathrm{el}} = \frac{\mu b^2}{2\pi(1-\nu)} \ln\left(\frac{x_0}{r_0}\right)$$

where x_0 is the distance between the opposite dislocations.

Remark - II

- In elastic energy because R enters into a logarithmic term, a change in its value has a little influence on the line energy

- For most uses $\ln(R/r_0)$ can be taken as 2π.

- It is convenient to approximate the elastic energy

$$E_{\mathrm{el}} = \frac{\mu b^2}{4\pi\kappa} \ln\left(\frac{R}{r_0}\right) \quad \Rightarrow \quad E_{\mathrm{el}} \approx \alpha \mu b^2$$

where $\alpha = 0.5 - 1$

Core Energy

- Ecore = energy of formation in a perfect crystal
- The core energy can be obtained only by rough approximation.

- These approximate evaluations suggest that the core energy is of the order of 1 eV/b, which is only a fraction of the elastic energy (1 eV = 1.6e-19 J)

- More accurate values can be drawn from first principles calculations

Further Reading

1. Argon, A.S., *Strengthening mechanism in crystal plasticity,* Oxford University Press, 2008.

2. Hirth, J.P., Lothe, J., *Theory of Dislocations*, 2nd ed., Wiley, 1982.

3. Kubin, L.P., *Dislocations, mesoscale simulations and plastic flow,* Oxford University Press, 2013.

4. Messerschmidt, U., *Dislocation Dynamics During Plastic Deformation*, Springer, 2010.