1 References

There are countless books about dislocations. The ones that I recommend are

- *Crystals, defects and micro-structures*, Rob Philips (Chap. 8).

2 Continuum theory of dislocations

Dislocations are line defects in crystals. Under normal conditions, they are the main carriers of plastic deformation, and therefore are crucial in its description. The defining property of a dislocation is that preforming a line integral over the displacement field around the dislocation line results in a non-zero value:

\[ \oint du_i = \oint \partial_j u_i dx_j \equiv b_i \neq 0 \]  

This value, \( \vec{b} \), is called the Burger’s vector of the dislocation.
2.1 Volterra model, elastic fields

The Volterra model for a dislocation consists of cutting a bulk along a half plane, and then shifting the relative parts (Fig 1a). The boundary of the half plane is called the dislocation line. If the displacement is parallel to the dislocation line, the dislocation is called screw dislocation and is similar to multi-stories parking lots. If the deformation is perpendicular to the dislocation line, it is called an edge dislocation. When both components are present the dislocation is called a mixed dislocation.

The discrete analogue of the continuum contour integral (1) can be thought of as walking along the crystalline directions in what is supposed to be a closed circle (Fig 1a, “10 atoms downwards, 10 to the right, 10 upwards and 10 left”). If the loop does not close, you have encircled a dislocation. Note that very close to the dislocation core it is hard to tell what are the crystalline axes, but far away there’s no problem. You also see that the direction and magnitude of the Burgers vector is related to the crystal structure.

The elastic fields of such a straight dislocation can be calculated. In fact, we’ve already preformed this calculation in class for screw dislocations (starting around Eq (5.45) in the lecture notes). If the dislocation line is defined as the $\hat{z}$ direction, then the fields are

$$u_z = \frac{b_z \theta}{2\pi},$$

$$\epsilon_{\theta z} = \frac{1}{r} \frac{\partial}{\partial \theta} u_z = \frac{b_z}{2\pi r},$$

$$\sigma_{\theta z} = \mu \epsilon_{\theta z} \frac{\mu b_z}{2\pi r},$$

and all other components vanish. $b_z$ is the $z$ component of the burgers vector. A similar but a tiny bit less elegant result can be obtained for the case of an edge dislocation. We’ll quote only the stresses:

$$\sigma_{rr} = \sigma_{\theta \theta} = \frac{\mu b_\perp \sin \theta}{2\pi r},$$

$$\sigma_{zz} = \frac{2\nu}{1 - \nu} \frac{\mu b_\perp \sin \theta}{2\pi r},$$

$$\sigma_{r \theta} = -\frac{1}{1 - \nu} \frac{\mu b_\perp \cos \theta}{2\pi r}$$

where $\theta$ is measured from the “extra plane” of the dislocation.

Since the theory is linear, for mixed dislocations we can simply add their screw and edge components.

2.2 Dislocation energy

Note that the fields diverge at $r \to 0$. This is clearly unphysical, and where the stress is too high linear elasticity breaks down and something else happens. Also, as always we have a short-length cutoff at length comparable to the lattice spacing. The region where the elastic solution is no longer valid is called the dislocation core, and is of the order of the lattice spacing. Note that since the total energy goes like $\log(r_{\text{max}}/r_{\text{min}})$ we need both upper and lower cutoffs - the system size and the dislocation core size. The dislocation energy diverges with the system size!
In the core, additional energy is stored which is not described by linear elasticity. As a crude estimate, we can say that the stress there is fixed at its value on the core radius \( r_c \), where \( r_c \) is the core’s radius (something like elastic-perfect-plastic behavior). The energy (per unit length) of the core is thus \( E_{\text{core}} = \mu \epsilon r_\theta \sigma r_\theta (\pi r_c^2) \). If we estimate \( r_c \sim b \), the total energy per unit length of the dislocation reads, roughly,

\[
E_{\text{tot}} / L \sim \mu b^2 \left( \log \frac{r_{\text{max}}}{b} + 1 \right)
\]  

(8)

For metals, typically \( \mu \sim 50\text{GPa} \), \( b \sim 1\text{Å} \). Even for very small systems, say \( r_{\text{max}} \sim 10\text{nm} \), and \( \log(\cdot) \sim 1 \), the energy is \( \mu b^2 \sim 4\text{-}5\text{ eV per nm} \). This is much larger than thermal energies at R.T. (\( k_B T \sim 1/40\text{eV} \)), so this raises serious questions about the nature of dislocations. They can not be created by thermal fluctuations - they are purely out-of-equilibrium creatures.

### 2.3 Deformation

Plastic deformation occurs when dislocations travel to the boundary of the material. In fact, the dislocation line can be thought of the boundary between the region along the slip plane that has slipped and the region that didn’t slip yet (again, Fig. 1a). When the dislocation reaches the boundary, an atomic step is created. Each dislocation carries with it a “deformation charge” equal to its Burgers vector. This is, in a way, a topological charge, that is conserved. Dislocation lines can split, coalesce, form junctions etc. but the Burgers vector is always conserved. A way to see this is that the deformation fields are continuous and therefore when deforming the integration contour (1) the result cannot change.

### 2.4 Forces, configurational forces and interactions

In order to investigate the interaction between dislocations and other stuff (external forces, other dislocations, free boundaries, point defects...) we need to look at the energy. For example, let’s consider two parallel edge dislocations with two parallel Burger vectors \( b_1, b_2 \) at distance \( d \) apart. The total energy of the system is

\[
E_{\text{tot}} = E_{\text{core}}^1 + E_{\text{core}}^2 + \int_\Omega \left( \epsilon_{ij}^1 + \epsilon_{ij}^2 \right) \left( \sigma_{ij}^1 + \sigma_{ij}^2 \right) d^3 x
\]

(9)

\[
= E_{\text{self}}^1 + E_{\text{self}}^2 + \int_\Omega \left( \epsilon_{ij}^1 \sigma_{ij}^2 + \epsilon_{ij}^2 \sigma_{ij}^1 \right) d^3 x
\]

(10)

The self energies are independent of \( d \). However, the interaction term does depend on \( d \), and its derivative with respect to \( d \) is the force that the dislocation exert on one another. These kind of forces – that is, derivatives of the energy with respect to a translational-symmetry-breaking parameter – are called configurational forces. The interaction energy (per unit length squared) is evaluated to be

\[
E_{\text{int}} = \frac{\mu b_1 b_2}{2\pi(1 - \nu)} \frac{1}{x - x'}
\]

(11)
The interaction is repulsive if the $b_1$ and $b_2$ have the same sign, and vice versa. This is a simple case where the dislocations are parallel and so is their Burgers vector - in the general case the interaction is highly anisotropic. We see that dislocations are very strongly interacting (interaction energy decays as $r^{-1}$). This is usually thought to induce strain hardening, etc (Fig. 1b).

Following the same procedure, we can calculate the interaction energy of a dislocation and an external stress field $\sigma$. Differentiating with respect to the position of the dislocation, we get the Peach-Koheler force:

$$\vec{F} = \varepsilon_{ijk} \sigma \xi \bar{b} \xi_j = (\sigma \bar{b}) \times \hat{\xi}$$

where $\vec{F}$ is the force per unit length and $\hat{\xi}$ is the direction of the dislocation line.

### 3 Discrete effects

#### 3.1 A “continuous” dislocation

![Figure 2: Setup for the calculation of the Peierls-Nabarro dislocation. From Hirth & Lothe. Note that here we assume that the magnitude of the Burgers vector is one lattice spacing.](image)

We’ve seen that there are configurational forces acting on dislocations (and other defects), but in order to get a notion about the plastic flow, we still need to say something about the dynamics of dislocation movement. When two dislocations interact and the energy is not at its minimum (i.e., there are forces), will the dislocation always move? And what about external forces?

For this, we need some model of the dislocation core. Probably the simplest model that offers good quantitative predictions is the Peierls-Nabarro model. The setup is sketched in Fig. 2: Assume we have two half-infinite lattices with the bottom lattice having an extra plane of atoms. Now glue the half lattices together. What will be the displacement field that minimized the energy? To each point along the slip plane we can assign a local
misregistry value $\Delta(x)$ which measures to what extent the crystals above and below the plane are misaligned. We know that $\Delta(\infty) = -\Delta(-\infty) = b/2$, and knowing the profile of $\Delta(x)$ is the goal.

The energy of the dislocation is composed of the elastic energy of the bulk, derived earlier, and additional term, $E_{mis}$ which is called the misfit energy and which stems from the inter-planar potential $\phi(\Delta)$. The potential has the same periodicity as the lattice. The misfit energy might be thought of as the core energy mentioned before. We write

$$E_{mis} = \int_{-\infty}^{\infty} \phi(\Delta(x)) dx$$

We now remind ourselves of Clapeyron’s theorem, which says that in static conditions the elastic energy stored in the bulk of a general solid is

$$E_{bulk} = \frac{1}{2} \int_{\partial \Omega} \sigma_{ij} u_j n_i$$

In our case, we’ll integrate on the two half-crystals above and below the slip plane. The normal is therefore $\hat{y}$, and we have two surfaces as $y = \pm \eta$ with $\eta \rightarrow 0$. The energy is

$$E_{bulk} = \frac{1}{2} \int_{-\infty}^{\infty} \sigma_{xy}(u_x(\eta) - u_x(-\eta)) dx = \frac{1}{2} \int_{-\infty}^{\infty} \sigma_{xy} \Delta(x) dx$$

For the Volterra dislocation, we use the stresses from (7):

$$\sigma_{xy}(y = 0) = \frac{\mu b^2}{2\pi(1-\nu)} \frac{1}{x}$$

and $\Delta(x)$ is simply

$$\Delta(x) = \begin{cases} 
  b & x < 0 \\
  0 & x > 0 
\end{cases}$$

so the energy is

$$E_{bulk} = \frac{1}{2} \int_{-\infty}^{0} \frac{\mu b^2}{2\pi(1-\nu)} \frac{1}{x}$$

and it is infinite. The misfit energy, however, is zero. Thus, we expect that the lattice will find a way to reduce the energy by “smoothing out” the dislocation core, whose size is zero in the Volterra model, thus increasing the misfit energy but reducing the bulk energy.

The key point in our modeling of the core is considering the slip plane as composed of a continuous distribution of infinitesimal parallel edge dislocations, with their magnitude given by $b(x) = (\partial_x \Delta) dx$, or density $\rho = \partial_x \Delta$. We’ll see that for a dislocation with “core density” $\rho(x)$ the stress field will not diverge: it is the convolution of Eq. (16) with $\rho$, i.e.,

$$\sigma_{xy}(x) = \frac{\mu}{2\pi(1-\nu)} \int_{-\infty}^{\infty} \frac{\rho(x')}{x - x'} dx'$$

In order to find the minimizer of the energy we can write the total energy and use the Euler-Lagrange Equations. This is a somewhat technical calculation which we will not
follow here. However, it’s final result is very intuitive: it simply states that the stresses induced by the dislocations should exactly cancel the effective stresses induced by the misfit energy, i.e.

\[ \phi'(\Delta) = \frac{\mu}{4\pi(1-\nu)} \int_{-\infty}^{\infty} \frac{\partial x' \Delta(x')}{x-x'} dx \]  

(20)

This is an integro-differential equation and to solve it, we need an explicit form for \( \phi \). Note that \( \phi \) must have the same symmetry of the lattice, and in particular in must be a periodic function with period \( d \). The simplest function that does that is a cosine,

\[ \phi(\Delta) = \phi_0 \left( 1 - \cos \frac{2\pi \Delta}{d} \right) \]  

(21)

where \( d \) is the inter-planar spacing. This form was also used in the derivation of the “ideal shear strength” (Eq. (11.5) in Eran’s notes). The constant \( \phi_0 \) can be obtained by demanding compliance with Hooke’s law: for small displacements the restoring stress must be

\[ \sigma_{xy} = 2\mu \varepsilon_{xy} = 2\mu \frac{\Delta}{d} + \mathcal{O}(\Delta^2) \]  

(22)

\[ \frac{\partial \phi}{\partial \Delta} = \frac{\pi \phi_0}{d} \sin \left( \frac{2\pi \Delta}{d} \right) = \frac{2\pi^2 \phi_0}{d^2} \Delta + \mathcal{O}(\Delta^2) \]  

(23)

and equating the two gives \( \phi_0 = \frac{\mu b^2}{\pi^2 d} \). With this form for the potential we arrive at the famous Peierls-Nabarro integro-differential equation

\[ \frac{\mu}{4\pi(1-\nu)} \int_{-\infty}^{\infty} \frac{\Delta'(x')}{x-x'} dx' = \frac{\phi_0 \pi}{d} \sin \frac{2\pi \Delta}{d} \]  

(24)

The solution of integro-differential equation is a whole story that we’re not getting into. The solution to this particular equation was given by Peierls to be

\[ \Delta(x) = \frac{b}{\pi} \tan^{-1} \left( \frac{x}{\zeta} \right) - \frac{b}{2}, \quad \zeta = \frac{\mu b^2}{4\pi^2 \phi_0 (1-\nu)} \]  

(25)

Note that the core half-width \( \zeta \) represents the competition between the elastic stiffness \( \mu \), which tends to spread the dislocations out, and the non-linear misfit potential \( \phi_0 \), which tends to localize the dislocation core. Plugging in our value for \( \phi_0 \) yields \( \zeta = \frac{d}{2(1-\nu)} \) and this confirms our estimation that the core width scales with the lattice spacing.