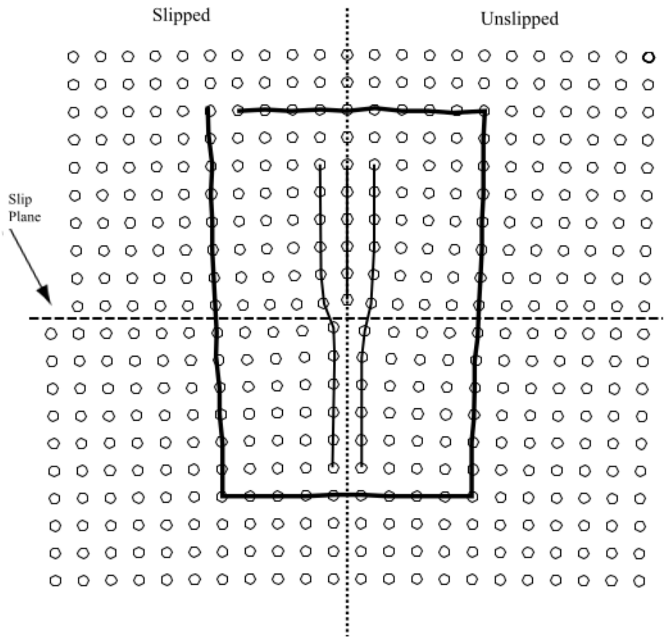
Dislocations

1 References

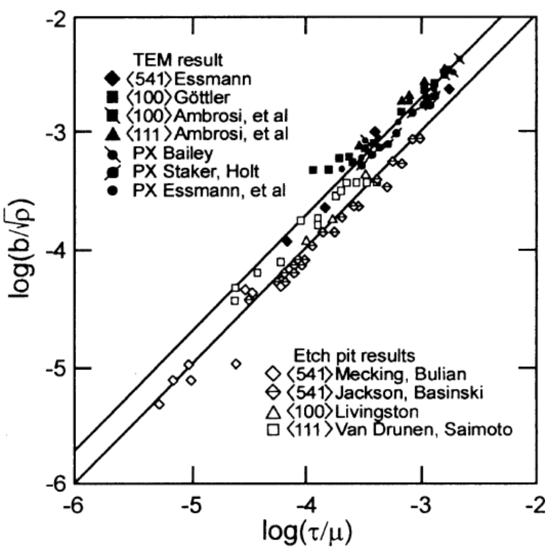
There are countless books about dislocations. The ones that I recommend are

- *Theory of dislocations*, Hirth & Lothe.
- *Crystals, defects and micro-structures*, Rob Philips (Chap. 8).
- *Elementary dislocation theory*, Weertman & Weertman.

2 Continuum theory of dislocations



(a) Schematic of a dislocation (From Rob Philips' book)



(b) Yield stress as a function of dislocation density (Kocks & Mecking, 2001).

Figure 1

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:

$$\oint du_i = \oint \partial_j u_i dx_j \equiv b_i \neq 0 \ , \tag{1}$$

this value, $\vec{b}$, is called the Burger's vector of the dislocation[1].

[1] Many sources define this integral as $-\vec{b}$, so be careful.

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*, See Fig. 2. When

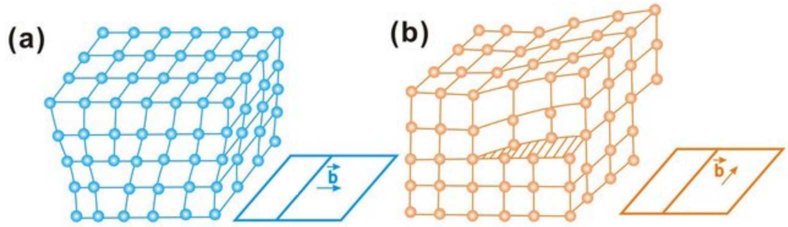


Figure 2: (a) Edge dislocation. (b) Screw dislocation.

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

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

$$\epsilon_{\theta z} = \frac{1}{2r}\partial_\theta u_z = \frac{b_z}{4\pi r} \,, \tag{3}$$

$$\sigma_{\theta z} = 2\mu\epsilon_{\theta z} = \frac{\mu b_z}{2\pi r} \,, \tag{4}$$

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:

$$\sigma_{rr} = \sigma_{\theta\theta} = \frac{\mu b_\perp}{2\pi(1-\nu)}\frac{\sin\theta}{r} \,, \tag{5}$$

$$\sigma_{zz} = \nu(\sigma_{rr} + \sigma_{\theta\theta}) = \frac{\nu\mu b_\perp}{\pi(1-\nu)}\frac{\sin\theta}{r} \,, \tag{6}$$

$$\sigma_{r\theta} = -\frac{1}{1-\nu}\frac{\mu b_\perp}{2\pi}\frac{\cos\theta}{r} \,, \tag{7}$$

where θ 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 $\log(r_{max}/r_{min})$ 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. The energy (per unit length) of the core of a screw dislocation is thus $E_{core} = \ \epsilon_{\theta z} \ \sigma_{\theta z}(\pi r_c^2) = \frac{\mu b_z^2}{8\pi}$. If we estimate $r_c \sim b_z$, the total energy per unit length of the dislocation reads, roughly,

$$E_{tot}/L = \frac{\mu b_z^2}{8\pi}\left(1 + 2\log\left(\frac{r_{\max}}{r_c}\right)\right) \sim \frac{\mu b_z^2}{8\pi}\left(1 + 2\log\left(\frac{r_{\max}}{b_z}\right)\right) \ . \tag{8}$$

For metals, typically $\mu \sim 50$GPa, $b \sim 1$Å. Even for very small systems, say $r_{max} \sim 10$nm, the energy ~ 1eV per nm. This is much larger than thermal energies at R.T. ($k_B T \sim 1/40$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 screw dislocations with two parallel Burger vectors b_1, b_2 at distance d apart. The total energy of the system is

$$\begin{aligned} E_{tot} &= E^1_{core} + E^2_{core} + \int_\Omega \left(\epsilon^1_{ij} + \epsilon^2_{ij}\right)\left(\sigma^1_{ij} + \sigma^2_{ij}\right) d^3x \\ &= E^1_{self} + E^2_{self} + \underbrace{\int_\Omega \left(\epsilon^1_{ij}\sigma^2_{ij} + \epsilon^2_{ij}\sigma^1_{ij}\right) d^3x}_{E_{int}} \ . \end{aligned} \tag{9}$$

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[2] (per unit length) is evaluated[3] to be

$$E_{int} = -\frac{\mu b_1 b_2}{2\pi} \log \left| \vec{r}_1 - \vec{r}_2 \right| \ . \tag{10}$$

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 (attraction/repulsion 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 $\boldsymbol{\sigma}$. Differentiating with respect to the position of the dislocation, we get the Peach-Koheler force:

$$\vec{F} = \mathcal{E}_{ijk} \sigma_{il} b_l \xi_j = (\boldsymbol{\sigma} \vec{b}) \times \hat{\xi} \ , \tag{11}$$

where $\vec{F}$ is the force per unit length and $\hat{\xi}$ is the direction of the dislocation line. A great example of a bunch of dislocations and their motions is seen (through a microscope) here.

3 Discrete effects

3.1 A "continuous" dislocation

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. 3: 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 $\Delta(\infty) - \Delta(-\infty) = b$, 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 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

[2] Actually, doing the integral noted gives rise to a more complicated term, but all the complications are constant, so we elegantly forget about them.

[3] In general, an argument inside a logarithm should be non-dimensional, but in this case it just gives rise to a constant energy, which isn't interesting.

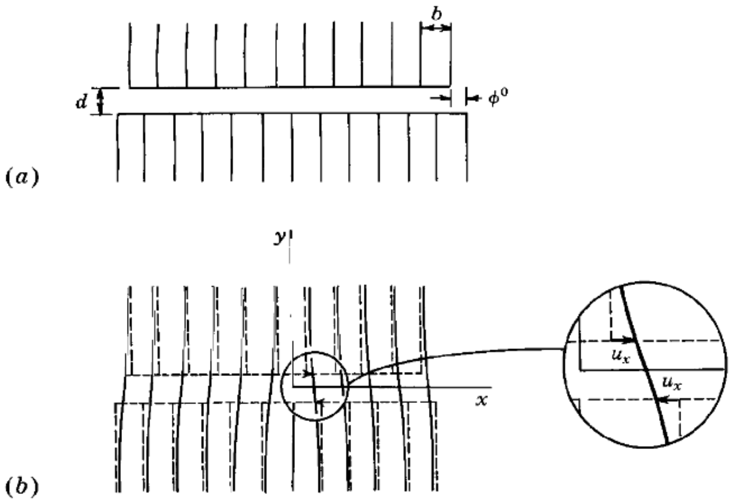


Figure 3: Setup for the calculation of the Peierls-Nabarro dislocation. From Hirth & Lothe. Note that here we assume that the magnitude of the Burgers vector is one lattice spacing.

lattice. The misfit energy might be thought of as the core energy mentioned before. We write

$$E_{mis} = \int_{-\infty}^{\infty} \phi(\Delta(x))dx \ . \tag{12}$$

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

$$E_{bulk} = \frac{1}{2} \int_{\partial\Omega} \sigma_{ij} u_j n_i \ . \tag{13}$$

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 $\eta \to 0$. The energy is

$$E_{bulk} = \frac{1}{2} \int_{-\infty}^{\infty} \sigma_{xy}(u_x(\eta) - u_x(-\eta))dx = \frac{1}{2} \int_{-\infty}^{\infty} \sigma_{xy} \Delta(x) dx \ . \tag{14}$$

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

$$\sigma_{xy}(y = 0) = \frac{\mu b}{2\pi(1-\nu)} \frac{1}{x} \ , \tag{15}$$

and $\Delta(x)$ is simply

$$\Delta(x) = b\Theta(x) \ , \tag{16}$$

where Θ is the Heaviside step function, so the energy is

$$E_{bulk} = \frac{b^2 \mu}{2\pi(1-\nu)} \int_0^{\infty} \frac{dx}{x} \ , \tag{17}$$

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. (15) with ρ, i.e.,

$$\sigma_{xy}(x) = \frac{\mu}{2\pi(1-\nu)} \int_{-\infty}^{\infty} \frac{\rho(x')}{x - x'} dx' \ . \tag{18}$$

In order to find the minimzer 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.

$$\phi'(\Delta) = \frac{\mu}{2\pi(1-\nu)} \int_{-\infty}^{\infty} \frac{\partial_{x'} \Delta(x')}{x - x'} dx \ . \tag{19}$$

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

$$\phi(\Delta) = \frac{\phi_0}{2} \left(1 - \cos \frac{2\pi\Delta}{b} \right) \ . \tag{20}$$

This form was also used in the derivation of the "ideal shear strength" (Eq. (12.5) in Eran's notes). The constant ϕ_0 can be obtained by demanding compliance with Hooke's law: for small displacements the restoring stress must be

$$\begin{aligned} \sigma_{xy} &= 2\mu\varepsilon_{xy} = \mu \frac{\Delta}{d} + \mathcal{O}(\Delta^2) \ , \\ \frac{\partial \phi}{\partial \Delta} &= \frac{\pi \phi_0}{b} \sin \left(\frac{2\pi\Delta}{b} \right) = \frac{2\pi^2 \phi_0}{b^2} \Delta + \mathcal{O}(\Delta^2) \ , \end{aligned} \tag{21}$$

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

$$\frac{\mu}{2\pi(1-\nu)} \int_{-\infty}^{\infty} \frac{\Delta'(x')}{x - x'} dx' = \frac{\phi_0 \pi}{b} \sin \frac{2\pi\Delta}{b} \ . \tag{22}$$

The solution of integro-differential equations is a whole story that we're not getting into. The solution to this particular equation was given by Peierls to be[4]

$$\Delta(x) = \frac{b}{\pi} \tan^{-1} \left(\frac{x}{\zeta} \right) + \frac{b}{2}, \qquad \zeta = \frac{\mu b^2}{4\pi^2 \phi_0 (1-\nu)} \ . \tag{23}$$

Note that the core half-width ζ represents the competition between the elastic stiffness μ, which tends to spread the dislocations out, and the non-linear misfit potential ϕ_0, which

[4] If you will try to check this solution, save yourself some banging of heads against walls are recall that $\tan^{-1}$ is a multiply defined function.

tends to localize the dislocation core. Plugging in our value for ϕ_0 yields $\zeta = \frac{d}{2(1-\nu)}$ and this confirms our estimation that the core width scales with the lattice spacing. Notice also that $\Delta(\infty) - \Delta(-\infty) = b$, as demanded.

To further investigate the dynamics, we want to look deeper into the effect of having a periodic lattice. When the dislocation moves, the far-field parts of the energy, the bulk contribution, is independent of the location of the dislocation line. In order to obtain the misfit energy corresponding to the Peierls dislocation and to determine the Peierls stress, the sum of the local misfit energy has to be done at the position of atoms rows parallel to the dislocation line. Indeed, the PN equation holds for an elastic continuous medium whereas $\Delta(x)$ can only be defined where an atomic plane is present. The misfit energy can be thus considered as the sum of misfit energies between pairs of atomic planes and can be written as:

$$E_{mis} = \sum_{n=-\infty}^{\infty} \phi(\Delta(nb - x_c))b \; . \tag{24}$$

Note that we're mixing continuum and discrete descriptions like vodka and tomato juice, but this is the fun part. The misfit energy now reads

$$\begin{aligned} E_{mis} &= \frac{\phi_0 b}{2} \sum_{n=-\infty}^{\infty} \left[1 - \cos\left(\frac{2\pi}{b}\left[\frac{b}{\pi}\tan^{-1}\left(\frac{nb - x_c}{\zeta}\right) + \frac{b}{2}\right]\right)\right] \\ &= \frac{\phi_0 b}{2} \sum_{-\infty}^{\infty} \left[1 + \cos\left(2\tan^{-1}\left(\frac{bn - x_c}{\zeta}\right)\right)\right] \; . \end{aligned} \tag{25}$$

We now use high-school trigonometric identities

$$\cos(\tan^{-1}(x)) = \frac{1}{\sqrt{1+x^2}}, \qquad \sin(\tan^{-1}(x)) = \frac{x}{\sqrt{1+x^2}}, \qquad \cos(2x) = \cos^2 x - \sin^2 x \; ,$$

to get

$$E_{mis} = \zeta^2 \phi_0 b \sum_{-\infty}^{\infty} \frac{1}{(bn - x_c)^2 + \zeta^2} = \frac{\pi\zeta\phi_0 \sinh\left(\frac{2\pi\zeta}{b}\right)}{\cosh\left(\frac{2\pi\zeta}{b}\right) - \cos\left(\frac{2\pi x_c}{b}\right)} \; . \tag{26}$$

Although this result is exact, understanding its properties is very problematic, especially as we would like its derivative w.r.t x_c. This nasty sum can be also calculated using Poisson's summation formula:

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} f(z) e^{2\pi i k z} dz \; , \tag{27}$$

which is used when to sum stuff that one suspects will be nicer in Fourier space. Thus:

$$\begin{aligned} E_{mis} &= \zeta^2 \phi_0 b \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{e^{2\pi i k z}}{(bz - x_c)^2 + \zeta^2} dz \\ &= \frac{\zeta^2 \phi_0}{b} \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{e^{2\pi i k z}}{(z - \frac{x_c}{b})^2 + \frac{\zeta^2}{b^2}} dz = \pi\zeta\phi_0 \sum_{k=-\infty}^{\infty} e^{\frac{2\pi}{b}(ikx_c - \zeta|k|)} \; . \end{aligned} \tag{28}$$

We've seen that ζ (the dislocation core radius) and b (the burgers vector) are both of the order of d their ratio is of order unity. Thus, we can take the only the first two terms in the exponent, yielding

$$E_{mis} \approx \pi\zeta\phi_0 \left(1 + 2e^{-\frac{2\pi\zeta}{b}} \cos\left(\frac{2\pi x_c}{b}\right)\right) \ . \tag{29}$$

This very important result means that a dislocation moves under a periodic potential – a series of wells – and when passing from one position to the next a barrier must be passed. This energetic barrier is called Peierls' barrier. The stress needed to move a dislocation is given by the derivative of this energy w.r.t x_c (another configurational force):

$$\tau_{PN} \approx \frac{\mu}{1-\nu} e^{-2\pi\frac{\zeta}{b}} \sin\left(\frac{2\pi x_c}{b}\right) \ , \tag{30}$$

where we also divided by b to get from force to stress. The maximal value of this stress, i.e. the barrier height, is $\frac{\mu}{1-\nu}e^{-2\pi\zeta/b}$ and is orders of magnitude less than μ. Note that this predicts that the necessary stress to move a dislocation is lowest for the crystallographic planes that have the largest inter-planar distance, a prediction which is verified experimentally.

We conclude with a question - this is the necessary stress needed to move a dislocation if it is straight and moves rigidly. But we've just learned that it's easier to move stuff in a non-rigid way rather than step by step. What do you think actually happens with dislocations?