**Plasticity**

# 1 Leftovers from last time: Peierls-Nabarro potential

I remind you that in the last TA we asked what is the form of a dislocation if you an take a continuum dislocation with Burgers vector $b$ and add a discrete atomic scale potential with periodicity $d$, which is

$$\phi(\Delta) = \frac{\phi_0}{2}\left(1 - \cos\frac{2\pi\Delta}{d}\right) , \qquad \phi_0 = \frac{\mu b^2}{\pi^2 d} . \tag{1}$$

The result was Peierls-Nabarro dislocation core model, where the relative displacement between the the upper and lower half-planes was given by

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

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. However, the misfit energy depends on it strongly because of the short-wavelength periodic nature of $\phi$. We denote the location of the "extra" plane by $x_c$, and postulate that we can make the substitution

$$E_{mis} = \int_{-\infty}^{\infty} \phi(\Delta(x))dx \quad \rightarrow \quad \sum_{n=-\infty}^{\infty} \phi(\Delta(nb - x_c))\Delta x \tag{3}$$

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

$$E_{mis} = \frac{\mu b^2}{4\pi^2 d}\sum_{n=-\infty}^{\infty}\left[1 - \cos\left(\frac{2\pi}{b}\left[\frac{b}{\pi}\tan^{-1}\left(\frac{x_c + nb}{\zeta}\right) - \frac{b}{2}\right]\right)\right]\Delta x \tag{4}$$

$$= \frac{\mu b^2}{4\pi^2 d}\sum_{-\infty}^{\infty}\left[1 + \cos\left(2\tan^{-1}\left(\frac{x_c + nb}{\zeta}\right)\right)\right]\Delta x \tag{5}$$

We now use high-school trigonometric identities

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

to get

$$E_{mis} = \frac{\mu b^2 \zeta^2}{2\pi^2 d}\sum_{-\infty}^{\infty}\frac{1}{\zeta^2 + (x_c + nb)^2} \tag{6}$$

This nasty sum can be calculated using Poisson's summation formula:

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} f(x) e^{2\pi i k x} dx \tag{7}$$

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

$$E_{mis} = \frac{\mu b^2 \zeta^2}{2\pi^2 d} \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{e^{2\pi i k n}}{\zeta^2 + (x_c + nb)^2} dn \tag{8}$$

$$= \frac{\mu \zeta^2}{2\pi^2 d} \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{e^{2\pi i k n}}{\frac{\zeta^2}{b^2} + (\frac{x_c}{b} + n)^2} dn = \frac{\mu \zeta b}{2\pi d} \sum_{k=-\infty}^{\infty} e^{-2\pi |k| (\frac{\zeta}{b} + i \frac{x_c}{b})} \tag{9}$$

We've seen that $\zeta$ (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

$$E_{mis} \approx \frac{\mu \zeta b}{2\pi d} \left[ 1 + e^{-2\pi\zeta/b} \cos\left( \frac{2\pi x_c}{b} \right) \right] \ . \tag{10}$$

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):

$$\tau_{PN} \approx \frac{\mu}{1-\nu} e^{-2\pi \frac{\zeta}{b}} \sin\left( \frac{2\pi x_c}{b} \right) \ . \tag{11}$$

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 $\mu$. 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 but rather step by step. What do you think actually happens with dislocations?

# 2 Plastic cavitation

*Note: This section appears in Eran's Lecture notes*

Before we continue our discussion of the physics of plastic deformation, let us consider another example, still in the framework of the elastic-perfect plastic model. Earlier in the course, we considered the problem of elastic cavitation in soft solids. Can we analyze a similar problem for hard solids?

The answer is definitely yes, such an analogous phenomenon exists for hard solids, though the physical processes is different; while for soft solids elastic deformation can be very large and lead to cavitation, hard solids show a limited range of elastic response and the origin of cavitation is plastic deformation. We follow the kinematic analysis leading to Eq. (7.50) in the lecture notes, which is reproduced here

$$\lambda_r = \left(1 + \frac{L^3 - \ell^3}{r^3}\right)^{2/3} , \tag{12}$$

where $\lambda_r$ is the radial stretch, $L$ is the radius of the undeformed cavity and $\ell$ is the radius of the deformed one. The logarithmic strain $\epsilon_r$ reads

$$\epsilon_r = \log \lambda_r = \frac{2}{3} \log\left(1 + \frac{L^3 - \ell^3}{r^3}\right) . \tag{13}$$

The force balance equation was also derived in class (Eq. 11.14):

$$\frac{d\sigma_r}{dr} + 2\frac{\sigma_r - \sigma_\theta}{r} = 0 . \tag{14}$$

and the boundary conditions are

$$\sigma_r(r = \ell) = 0 \quad \text{and} \quad \sigma_r(r \to \infty) = \sigma^\infty . \tag{15}$$

Since symmetry implies $\sigma_\theta = \sigma_\phi$ and we assume incompressibility, the stress state is essentially uniaxial and we can write down a general constitutive law as

$$\sigma_r - \sigma_\theta = \sigma_y f(\epsilon_r) . \tag{16}$$

We then have

$$\begin{aligned} \int_\ell^\infty d\sigma_r &= -2\sigma_y \int_\ell^\infty \frac{f(\epsilon_r)dr}{r} = -2\sigma_y \int_\ell^\infty f\left[\frac{2}{3}\log\left(1 + \frac{(L/\ell)^3 - 1}{(r/\ell)^3}\right)\right] \frac{d(r/\ell)}{(r/\ell)} \\ \Longrightarrow \sigma^\infty &= -2\sigma_y \int_1^\infty f\left[\frac{2}{3}\log\left(1 + \frac{(L/\ell)^3 - 1}{x^3}\right)\right] \frac{dx}{x} . \end{aligned} \tag{17}$$

Where we introduced the dimensionless variable $x = r/\ell$. The cavitation threshold $\sigma_c$ is defined as the stress needed to grow the cavity indefinitely, i.e. $\ell \gg L$. This leads to

$$\sigma_c = \lim_{\ell\to\infty} \sigma^\infty = -2\sigma_y \int_1^\infty f\left[\frac{2}{3}\log\left(1 - x^{-3}\right)\right] x^{-1} dx . \tag{18}$$

We now need to choose a constitutive law $(\sigma_r - \sigma_\theta)/\sigma_y = f(\epsilon_r)$. For this demonstration, we choose an elastic-perfect-plastic material:

$$\begin{aligned} \sigma &= E\epsilon \quad \text{for} \quad \epsilon < \frac{\sigma_y}{E} \\ \sigma &= \sigma_y \quad \text{for} \quad \epsilon \geq \frac{\sigma_y}{E} . \end{aligned} \tag{19}$$

which we interpret here as pertaining to the logarithmic strain and also allow all quantities to be signed,

$$\begin{aligned} f(\epsilon_r) &= \frac{\epsilon_r}{\epsilon_y} \quad \text{for} \quad |\epsilon_r| < \epsilon_y \\ f(\epsilon_r) &= \text{sign}(\epsilon_r) \quad \text{for} \quad |\epsilon_r| \geq \epsilon_y , \end{aligned} \tag{20}$$

where $\epsilon_y \equiv \sigma_y/E$. With this law at hand, after a few rather simple mathematical manipulations, we obtain a nice analytic result. First, we use the yield strain $\epsilon_y$ inside the argument of $f(\cdot)$ in the above integral

$$-\epsilon_y = \frac{2}{3}\log\left(1 - x_y^{-3}\right) \Longrightarrow x_y = \left[1 - \exp(-3\epsilon_y/2)\right]^{-1/3} \ . \tag{21}$$

This allows us to use the constitutive law in order to split the integral into its elastic and plastic contributions as

$$\frac{\sigma_c}{\sigma_y} = \underbrace{2\int_1^{x_y} x^{-1}dx}_{\text{Plastic domain}} \underbrace{- \frac{4}{3\epsilon_y}\int_{x_y}^{\infty} \log\left(1 - x^{-3}\right) x^{-1}dx}_{\text{Elastic domain}} \ . \tag{22}$$

We now recall that there exists a small parameter in the problem, $\epsilon_y \ll 1$ (since for ordinary hard solids the yield stress is much smaller than the elastic modulus). Therefore:

$$x_y \simeq \left(\frac{2}{3\epsilon_y}\right)^{1/3} \gg 1 \tag{23}$$

$$\log\left(1 - x^{-3}\right) \simeq -x^{-3} \qquad \text{for } x > x_y \text{, i.e. in the elastic domain .} \tag{24}$$

This immediately yields

$$\frac{\sigma_c}{\sigma_y} \simeq 2\log(x)\Big|_1^{\left(\frac{2}{3\epsilon_y}\right)^{1/3}} - \frac{4}{3\epsilon_y} \times \frac{x^{-3}}{3}\Big|_{\left(\frac{2}{3\epsilon_y}\right)^{1/3}}^{\infty} = \frac{2}{3}\log\left(\frac{2}{3\epsilon_y}\right) + \frac{2}{3} \ . \tag{25}$$

Therefore,

$$\frac{\sigma_c}{E} \simeq \frac{2\epsilon_y}{3}\left[1 + \log\left(\frac{2}{3\epsilon_y}\right)\right] \ . \tag{26}$$

As expected, $\sigma_c$ is an increasing function of $\sigma_y$ (for a fixed $E$), but the dependence is not trivial and could not have been guessed to begin with. This is an example of unlimited plastic flow under a fixed applied stress ("plastic collapse").

# 3 Unloading, residual stresses, shakedown (auto-frettage)

We consider a cylindrical shell under internal pressure. A very similar problem but in spherical geometry was fully solved by Eran, so we will not redo the calculation here. Instead, we will simply state the results. The solution under plane-strain conditions and the Tresca Criterion (HW) in the elastic region $c < r < b$ is

$$\sigma_{rr} = \sigma_y\left(\frac{c^2}{b^2} - \frac{c^2}{r^2}\right) \ . \qquad \sigma_{\theta\theta} = \sigma_y\left(\frac{c^2}{b^2} + \frac{c^2}{r^2}\right) \ , \tag{27}$$

and in the plastic region $a < r < c$ it is

$$\sigma_{rr} = \sigma_y\left[\frac{c^2}{b^2} - \log\left(\frac{c^2}{r^2}\right) - 1\right] \ , \qquad \sigma_{\theta\theta} = \sigma_y\left[\frac{c^2}{b^2} - \log\left(\frac{c^2}{r^2}\right) + 1\right] \ , \tag{28}$$

Since we are in plane-strain conditions, we the $zz$ component of the stress is given by $\sigma_{zz} = \nu(\sigma_{rr} + \sigma_{\theta\theta})$. In addition, we also have

$$p_c = \sigma_{rr}(r=c) = \sigma_y \left(1 - \frac{c^2}{a^2}\right) \quad , \qquad p_E = \sigma_y \left(1 - \frac{a^2}{b^2}\right) \quad , \qquad p_U = \sigma_y \log \frac{b^2}{a^2} \ , \tag{29}$$

and $c$ satisfies

$$\frac{p}{\sigma_y} = 1 - \frac{b^2}{c^2} + \log \frac{c^2}{a^2} \ . \tag{30}$$

Now, what happens if we remove the internal pressure? How do we deal with this kind of (un)loading? What is the constitutive law that one should use?

This is a tricky subject and there are many subtleties in the general case. In our case of perfect plasticity you can think about it in the following manner: The perfect plastic constitutive law makes sure that the stress state at any given point in the material will always be inside the yield surface (in the elastic case) or strictly on it (in the plastic case). In other words, every point which is in a plastic state is also exactly on the threshold of yielding. Thus, the unloading dynamics is governed by elasticity. Or more precisely, as we'll soon see, at least the first part of it is governed by elasticity.

So we conclude that to get the unloaded state we need to subtract the fully elastic solution from the elasto-plastic solution. That is, we need to subtract Eq. (27) with $c \to a$ and $\sigma_y \to p/(\frac{b^2}{a^2} - 1)$ from (28). The result is

$$\begin{aligned} \sigma_{rr} &= -\sigma_y \left(\frac{c^2}{a^2} - \frac{p}{p_E}\right)\left(\frac{a^2}{r^2} - \frac{a^2}{b^2}\right) \\ \sigma_{\theta\theta} &= \quad \sigma_y \left(\frac{c^2}{a^2} - \frac{p}{p_E}\right)\left(\frac{a^2}{r^2} + \frac{a^2}{b^2}\right) \end{aligned} \qquad c < r < b \tag{31}$$

$$\begin{aligned} \sigma_{rr} &= -\sigma_y \left[\frac{p}{p_E}\left(1 - \frac{a^2}{r^2}\right) - \log \frac{r^2}{a^2}\right] \\ \sigma_{\theta\theta} &= -\sigma_y \left[\frac{p}{p_E}\left(1 + \frac{a^2}{r^2}\right) - \log \frac{r^2}{a^2} - 2\right] \end{aligned} \qquad a < r < c \tag{32}$$

Note that the system has no tractions at the boundaries but the stress field does not vanish! These stresses are called residual stresses. The largest value of $|\sigma_{\theta\theta} - \sigma_{rr}|$ is at $r = a$, where it is $2\sigma_y(p/p_E - 1)$. Unloading is thus purely elastic if $p/p_E \le 2$. This is surely the case if $p_U < 2p_E$. That is, if

$$\sigma_y \log \frac{b^2}{a^2} < 2\sigma_y \left(1 - \frac{a^2}{b^2}\right) \tag{33}$$

The condition (33) is satisfied if $b/a \le 2.218$. If, on the other hand, $p < 2p_E$ then the unloading itself will create a new plastic zone at $a < r < c'$.

We can therefore define $p_s = \min(2p_E, p_U)$ ($s$ for shakedown). If $p < p_S$ then unloading is elastic, and *every subsequent loading/unloading with pressure up to $p$ is also elastic!*.

Physically, the portions of the cylinder that have underwent plastic deformation are now providing additional hoop stresses to the cylinder, making it stronger than it was before the plastic flow. In the context of reinforcing metal cylinders so that they can withstand high internal pressures (you can guess what is the technological motivation for that) this is called auto-frettage ("frettage" is French for the process of putting hoops). In a more general context this is called "shakedown". A similar concept is used in reinforced concrete.