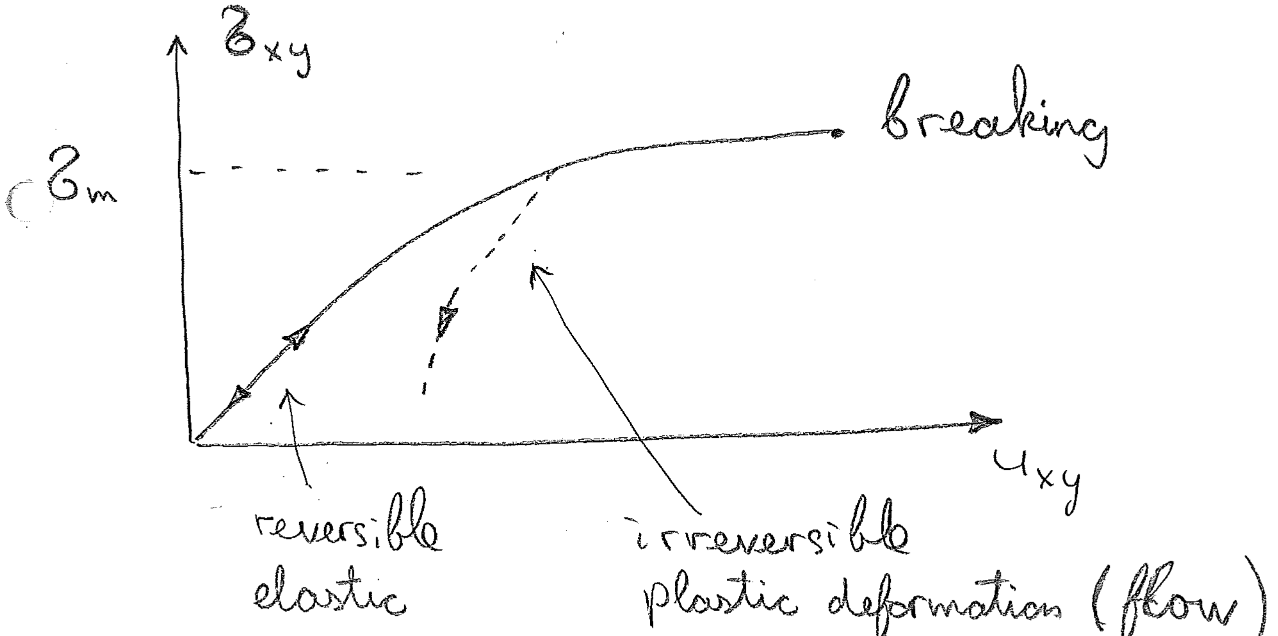
Lecture 2 (1)

Dislocations

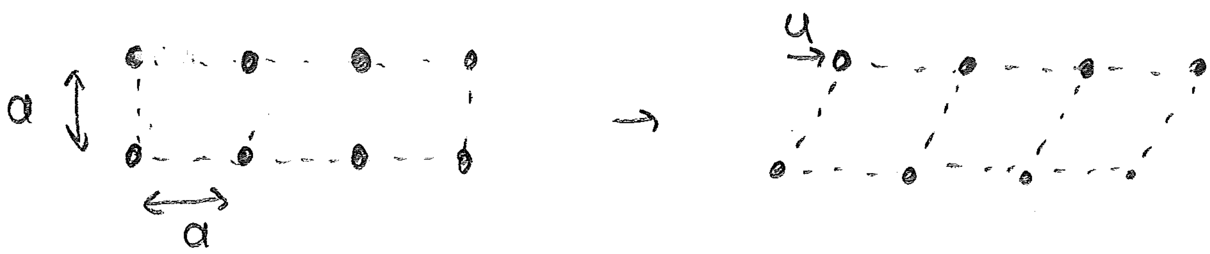
Hooke's law is linear response law.

With increase of deformation stress-strain relation becomes nonlinear



Let us estimate the yield stress σ_m that solid can sustain without breaking or flowing

We should take into account periodic structure of crystal.



For small u the strain is $\frac{u}{a}$ and stress is $\mu \frac{u}{a}$.

When atoms are shifted by a period a crystal goes to undeformed state.

It is natural to assume that the stress σ is a periodic function of u

$$\sigma \propto \sin \frac{2\pi u}{a}$$

Since it should go to $\sigma = \mu \frac{u}{a}$ for $u \ll a$ we can write it as

$$\sigma = \frac{\mu}{2\pi} \sin \frac{2\pi u}{a}$$

That gives the maximal stress

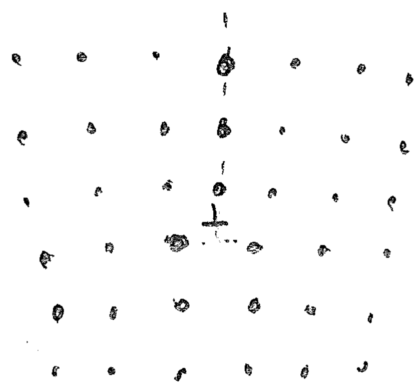
$$\sigma_m = \frac{\mu}{2\pi} \simeq \frac{\mu}{10}$$

In reality yield stresses are much lower $\sim 10^{-4}\mu$

Why ?

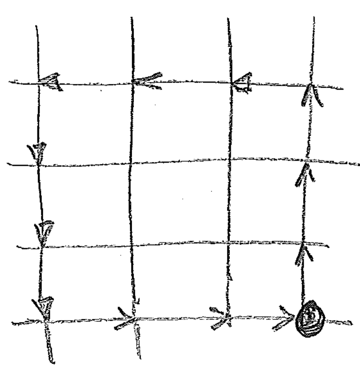
This is due to special defects called <u>dislocations</u>.

<u>Edge</u> dislocation looks like additional half plane inserted in the crystal

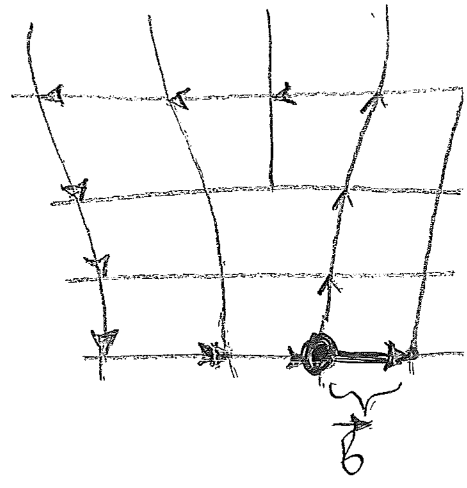


One can define it in the following way

Consider any closed path in an ideal crystal following nearest neighbor bonds in the lattice

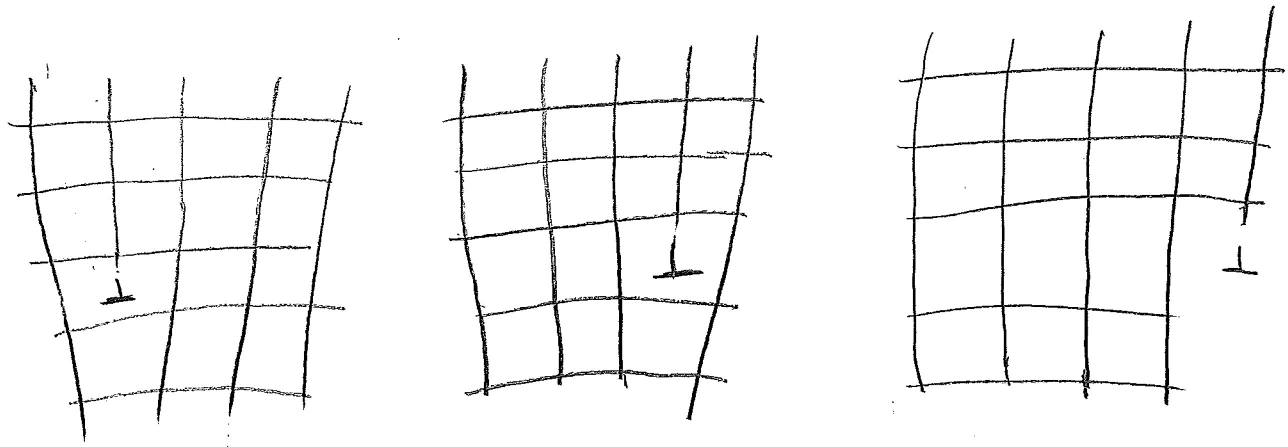


The same sequence of steps around dislocation will lead to displacement $\vec{b}$



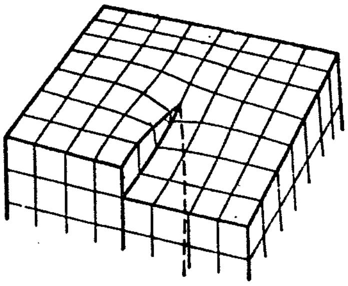
This vector $\vec{b}$ is called <u>Burgers vector</u>

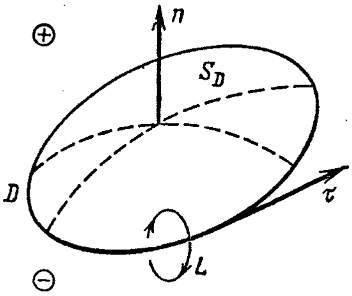
The Burgers vector doesn't depend on the chosen path $\Rightarrow$ dislocation is topological defect. Although far away from its <u>core</u> deformations are small, by going around we can see that defect is present.

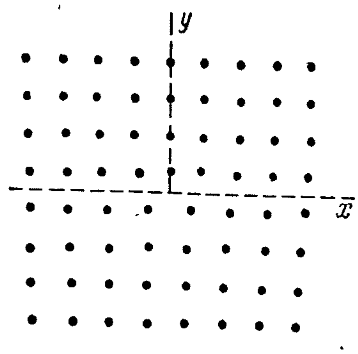


If dislocation moves through the crystal it produces shift of the upper half crystal by the unit vector $\vec{b}$. The shear that leads to the dislocation motion is much smaller than μ. That is why $\sigma_m << \mu$

2 Dislocations







$$\oint du_i = \oint \frac{\partial u_i}{\partial x_k} dx_k = -b_i \qquad (1)$$

$\vec{b}$ is called <u>Burgers vector</u>

For the screw dislocation $\vec{b} \parallel \vec{\tau}$

For the edge dislocation $b \perp \vec{\tau}$

$\vec{\tau}$ is the tangent vector at the given point of the dislocation.

In general case dislocation line is a curve along which the angle between $\vec{b}$ and $\vec{\tau}$ is changing. Burgers vector, however, doesn't change along the dislocation line.

Because of topological nature of Eq. (1) dislocation can not end inside the sample.

Displacement field

Eq. (1) means that in the presence of a dislocation displacement vector $\vec{u}(r)$ is a multivalued function. However, since $\vec{b}$ is equal to one of the lattice periods, displacement by $\vec{b}$ doesn't change the state of the lattice. Derivatives of $\vec{u}$, strain and stress tensors u_{ik}, σ_{ik} are single valued.

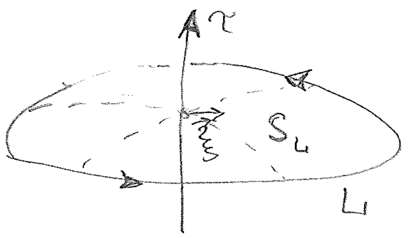
It is useful to introduce distorsion tensor

$$w_{ik} = \frac{\partial u_k}{\partial x_i} \qquad (\text{non symmetric})$$

$$u_{ik} = \frac{1}{2}(w_{ik} + w_{ki})$$

Eq. (1) can be rewritten as

$$\oint_L w_{ik}\, dx_i = -b_k$$



We can transform contour integral to the surface integral

$$\oint_L w_{ik}\, dx_i = -b_k = \int_{S_L} e_{ilm} \frac{\partial w_{mk}}{\partial x_l}\, dS_i$$

Since e_{ilm} is antisymmetric and $\dfrac{\partial w_{mk}}{\partial x_l} = \dfrac{\partial^2 u_k}{\partial x_l \partial x_m}$

is symmetric, $e_{ilm}\frac{\partial w_{mk}}{\partial x_e} \equiv 0$ everywhere apart from the crossing point of the dislocation line with the surface S_L (where w_{ik} is singular).

To define w_{ik} there

$$-b_k = \int e_{ilm}\frac{\partial w_{mk}}{\partial x_e}\, dS_i \Rightarrow e_{ilm}\frac{\partial w_{mk}}{\partial x_e} = -\tau_i b_k \delta^2(\vec{\xi})$$

or

$$\frac{\partial w_{nk}}{\partial x_k} - \frac{\partial w_{kk}}{\partial x_n} = -[\vec{\tau}\times\vec{b}]_n\, \delta^2(\vec{\xi}) \qquad (2)$$

Equilibrium equation $\frac{\partial \sigma_{ik}}{\partial x_k} = 0$ reads

$$\frac{\partial u_{ik}}{\partial x_k} + \frac{\sigma}{1-2\sigma}\frac{\partial u_{ee}}{\partial x_i} = 0$$

which can be rewritten through w_{ik}

$$\frac{1}{2}\frac{\partial w_{ik}}{\partial x_k} + \frac{1}{2}\frac{\partial w_{ki}}{\partial x_k} + \frac{\sigma}{1-2\sigma}\frac{\partial w_{ee}}{\partial x_i} = 0$$

Substituting condition (2) we obtain

$$\frac{\partial w_{ki}}{\partial x_k} + \frac{1}{1-2\sigma}\frac{\partial w_{ee}}{\partial x_i} = [\vec{\tau}\times\vec{b}]_i\,\delta^2(\vec{\xi})$$

$$\Downarrow$$

$$\Delta\vec{u} + \frac{1}{1-2\sigma}\,\mathrm{grad}\,\mathrm{div}\,\vec{u} = [\vec{\tau}\times\vec{b}]\,\delta^2(\vec{\xi})$$

Screw dislocation

$\vec{u}(x,y) \parallel z$ $\qquad \uparrow \vec{\tau}, \vec{b}_z$

$\Downarrow$

$\operatorname{div} \vec{u} = 0 \Rightarrow \Delta u_z = 0 \Rightarrow u_z = \frac{b}{2\pi} \varphi$

$u_{z\varphi} = \frac{b}{4\pi r}$, $\sigma_{z\varphi} = \frac{\mu b}{2\pi r}$. Other components $= 0$
(pure shear)

Energy of dislocation per length is

$$E = \frac{1}{2} \int \sigma_{ik} u_{ik} d^2 r = \frac{1}{2} \int 2 u_{z\varphi} \sigma_{z\varphi} d^2 r =$$

$$= \frac{\mu b^2}{4\pi} \int \frac{dr}{r} = \frac{\mu b^2}{4\pi} \ln \frac{R}{b}$$

Upper cut off R is either the system size or the size of the dislocation loop.

Edge dislocation $\vec{b} \parallel \vec{x}$

Equation for displacement is

$$\Delta u + \frac{1}{1-2\sigma} \nabla \operatorname{div} \vec{u} = -b \vec{e}_y \delta^2(r)$$

Let us look for a solution in form

$\vec{u} = \vec{u}_0 + w$ with $\vec{u}_0$: $u_x^0 = \frac{b}{2\pi} \varphi$, $u_y^0 = \frac{b}{2\pi} \ln r$

(This $\vec{u}_0 = \left(\operatorname{Im} \frac{b}{2\pi} \ln(x+iy), \operatorname{Re} \frac{b}{2\pi} \ln(x+iy) \right)$ satisfies Eq (1))

Thus w is singlevalued function

Since $\operatorname{div} \vec{u}_0 = 0$, $\Delta u_0 = b e_y \delta^2(r)$ $\Rightarrow$

w satisfies

$$\Delta w + \frac{1}{1-2\sigma} \nabla \operatorname{div} w = -2b\vec{e}_y \delta^2(r)$$

(Going to the Fourier space

$$k^2 \vec{w} + \frac{1}{1-2\sigma} \vec{k} (\vec{k} \cdot \vec{w}) = \vec{f} = -2b\vec{e}_y$$

$$\vec{w} = \frac{1}{k^2} \left(\vec{f} - \frac{\vec{k} \cdot (\vec{k} \cdot \vec{f})}{k^2} \frac{1}{2(1-\sigma)} \right) \Rightarrow$$

$$w = \frac{b}{4\pi(1-\sigma)} \int \left[\frac{(3-4\sigma)\vec{e}_y}{R} + \frac{\vec{r}\, y}{R^3} \right] dz', \quad R = \sqrt{r^2 + z'^2}$$

As a result we get

$$u_x = \frac{b}{2\pi}\left\{ \operatorname{arctg}\frac{y}{x} + \frac{1}{2(1-\sigma)}\frac{xy}{x^2+y^2}\right\}$$

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

Stress tensor is $\left(B = \frac{\mu}{2\pi(1-\sigma)}\right)$

$$\sigma_{xx} = -bB\frac{y(3x^2+y^2)}{(x^2+y^2)^2}, \quad \sigma_{yy} = bB\frac{y(x^2-y^2)}{(x^2+y^2)^2}, \quad \sigma_{xy} = bB\frac{x(x^2-y^2)}{(x^2+y^2)^2}$$

or $\sigma_{rr} = \sigma_{\varphi\varphi} = -bB\frac{\sin\varphi}{r}, \quad \sigma_{r\varphi} = bB\frac{\cos\varphi}{r}$

Energy of the dislocation is

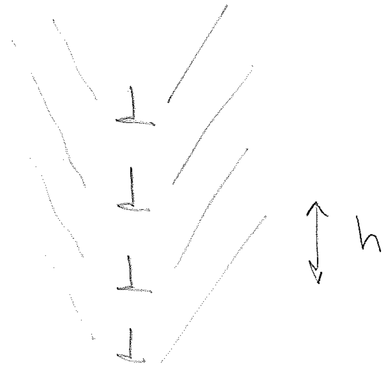
$$E = \frac{\mu b^2}{4\pi^2(1-\sigma)}\int \frac{y^2}{r^4}\,d^2r = \frac{\mu b^2}{4\pi(1-\sigma)}\ln\left(\frac{R}{b}\right)$$

Another derivation

Because of Eq.(1) we can define $\vec{u}$ as continuous function on a plane with cut surface S_e $\left.\vec{u}_+ - \vec{u}_-\right|_{S_e} = \vec{b}$. Then $F = \frac{1}{2}\int d^2r\,\sigma_{ij}u_{ij} = \frac{1}{2}\int d^2r\,\sigma_{ij}\nabla_j u_i$

$$= \frac{1}{2}(u_i^+ - u_i^-)\int \sigma_{ij}\,dS_j = \frac{1}{2}b\int_0^R \sigma_{xy}(\varphi=0)\,d\rho$$

Dislocation wall



$$\sigma_{xy}(x,y) = bBx \sum_{n=-\infty}^{\infty} \frac{x^2-(y-nh)^2}{\left[x^2+(y-nh)^2\right]^2}$$

We can rewrite it as

$$\sigma_{xy} = -bB\frac{\alpha}{h}\left[J(\alpha,\beta) + \alpha\frac{\partial J}{\partial \alpha}(\alpha,\beta)\right], \quad \alpha = \frac{x}{h}, \quad \beta = \frac{y}{h},$$

and $J(\alpha,\beta) = \sum_{-\infty}^{\infty} \frac{1}{\alpha^2+(\beta-n)^2}$

Using Poisson formula $\sum_{-\infty}^{\infty} f(n) = \sum_{k=-\infty}^{\infty} \int f(x)\, e^{2\pi i k x}\, dx$

we obtain

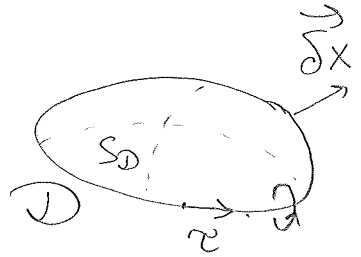
$$J(\alpha,\beta) = \int_{-\infty}^{\infty} \frac{d\xi}{\alpha^2+\xi^2} + 2\,\mathrm{Re}\sum_{1}^{\infty} e^{2\pi i k\beta} \int_{-\infty}^{\infty} \frac{e^{2\pi i k\xi}}{\alpha^2+\xi^2}\, d\xi =$$

$$= \frac{\pi}{\alpha} + \frac{2\pi}{\alpha}\sum_{1}^{\infty} e^{-2\pi k\alpha}\cos 2\pi k\beta$$

For $\alpha = \frac{x}{h} \gg 1$ only the first term in the sum survives and stress is decaying exponentially fast

$$\sigma_{xy} = 4\pi^2 B\,\frac{bx}{h^2}\, e^{-2\pi\frac{x}{h}} \cos\left(2\pi\frac{y}{h}\right)$$

Dislocation motion



S_D - surface where displacement jumps $\vec{u}_+ - \vec{u}_- \big|_{S_D} = \vec{b}$

Dislocation motion produces the change of S_D. With displacement $\delta\vec{x}$, the change of the surface

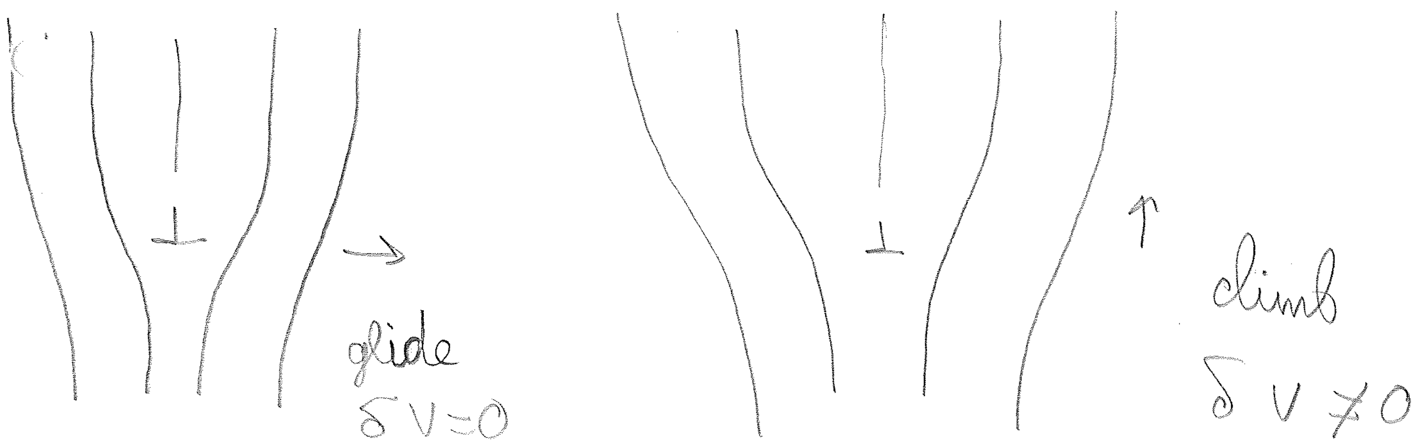
$$\delta S = [\delta\vec{x} \times d\vec{l}] = [\delta\vec{x} \times \vec{\tau}]\, dl$$

The change of volume of the medium is

$$\delta V = \vec{b} \cdot \delta\vec{S} = \delta\vec{x} \cdot [\vec{\tau} \times \vec{b}]\, dl$$

Two different situations:

Volume is unchanged if the motion is in the gliding plane $\parallel \tau, b$



glide is easy motion

climb - very hard due to diffusion of the point defects

Forces acting on dislocation

On the surface S_D $\vec{u}_+ - \vec{u}_- = \vec{b}$

Thus w_{ik} has these singularity

$$w_{ik}^{(s)} = n_i b_k \delta(\xi)$$

$\vec{n}$ is normal to the surface $\vec{\xi} \parallel \vec{n}$

$$u_{ik}^{(s)} = \frac{1}{2}(n_i b_k + n_k b_i)\,\delta(\xi)$$

Since due to dislocation motion S_D is changing

then by moving dislocation by $\delta\vec{r}$

$$\delta u_{ik}^{(pl)} = \frac{1}{2}\left\{ b_i [\vec{\delta r} \times \vec{\tau}]_k + b_k [\vec{\delta r} \times \vec{\tau}]_i \right\} \delta^2(r - r_d) \quad (3)$$

This is <u>plastic deformation</u>

Related with this deformation work due to external source is

$$\delta R = \int \sigma_{ik}^{ext}\, \delta u_{ik}\, dV$$

Substituting Eq. (3) we obtain

$$\delta R = \oint \sigma_{ik}^{ext}\, e_{ilm}\, \delta r_l\, \tau_m b_k\, dl$$

Thus we obtain the Peach Köhler force

$$\underline{f_i = e_{ikl}\, \tau_k\, \sigma_{lm}\, b_m}$$

Interaction of two edge dislocations

$\perp \, b_2$ $\qquad\qquad \tau_z = -1 \quad b_x = b$

$\perp \, b_1$

$$f_i = e_{ikl}\, \tau_k\, \sigma_{lm}\, b_m \Rightarrow$$

$$f_x = b\, \sigma_{xy} \;, \quad f_y = -b\, \sigma_{xx}$$

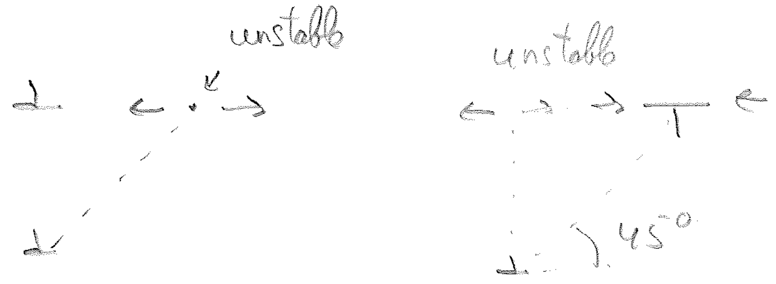
Using expressions for the stress around the edge dislocation we obtain

$$f_x = b_1 b_2 B \, \frac{x(x^2-y^2)}{r^4}$$

$$f_y = b_1 b_2 B \, \frac{y(3x^2+y^2)}{r^4} \qquad B = \frac{\mu}{2\pi(1-\nu)}$$

$$f_r = \frac{b_1 b_2 B}{r} \;, \quad f_\varphi = \frac{b_1 b_2 B}{r} \sin 2\varphi$$

Stable position



In the same glide plane two opposite dislocations attract each other

$\boxed{\text{1. Problem}}$ Calculate interaction of two screw dislocations

Peierls – Nabarro force

In continuum approximation dislocation can glide freely in the gliding plane.
But due to the discreteness of the atomic structure there is a finite barrier (Peierls barrier)
To calculate let us take discret version of

$$E = \frac{\mu b^2}{4\pi^2(1-\nu)}\, b^2 \sum_{nm} \frac{y_m^2}{\left((x-nb)^2+y_m^2\right)^2} =$$

$$= -\frac{\mu b^4}{4\pi^2(1-\nu)} \sum_m y_m^2 \frac{\partial}{\partial y_m^2} \sum_n \frac{1}{(x-nb)^2+y_m^2}$$

using again Poisson's formula

$$E = -\frac{\mu b^4}{4\pi^2(1-\nu)} \sum_m y_m^2 \frac{\partial}{\partial y_m^2} \sum_K \int \frac{e^{i2\pi kt}}{(x-tb)^2+y_m^2}\, dt =$$

$$= -\frac{\mu b^3}{4\pi^2(1-\nu)} \sum_m y_m^2 \frac{\partial}{\partial y_m^2} \sum_k \frac{\pi}{b\, y_m} \cos\frac{2\pi x k}{b}\, e^{-\frac{2\pi k y_m}{b}}$$

taking only the first term

$$E = \frac{\mu b^2}{4(1-\nu)} \cos\frac{2\pi x}{b}\, e^{-\frac{2\pi y_m}{b}}$$

Force

$$F = \frac{\pi \mu b}{2(1-\nu)} \sin\frac{2\pi x}{b}\, e^{-\frac{2\pi y_m}{b}}$$

In our case $y_m = \frac{b}{2}$ and critical stress $\sim \mu e^{-\pi}$. In "more" accurate model $y_m \approx b$

Usually critical stress $\sim 10^{-4}\mu$

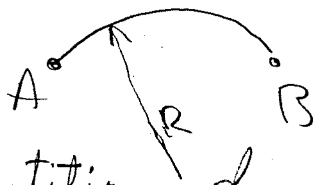
Problem 2. What is larger

e^{π} or π^{e}, find without computer

Frank - Read source

Consider dislocation fixed in 2 points (by impurities or by crossing with others dislocations in the network)

If there is stress => force on dislocation

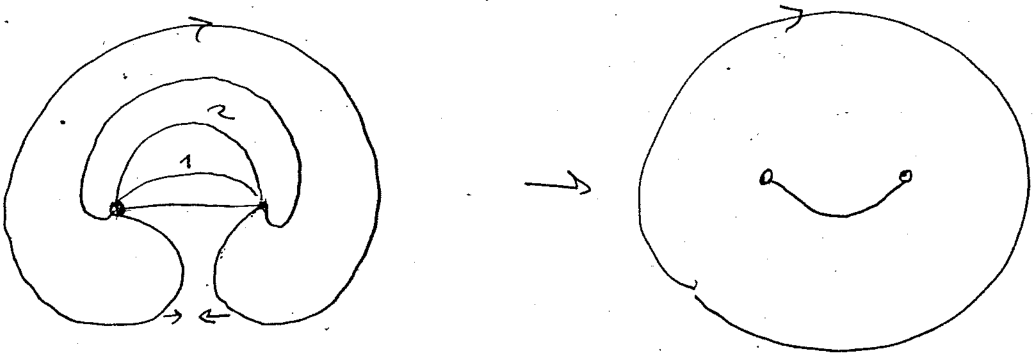


Equilibrium shape due to the competition of elasticity and force => circular shape

line tension of dislocation $\sim \mu b^2$

$$f = \frac{\varepsilon_e}{R}$$

with increasing force R decreases



for $f > \dfrac{\varepsilon_e}{|AB|}$ loop expands cuts and we get free loop + original dislocation