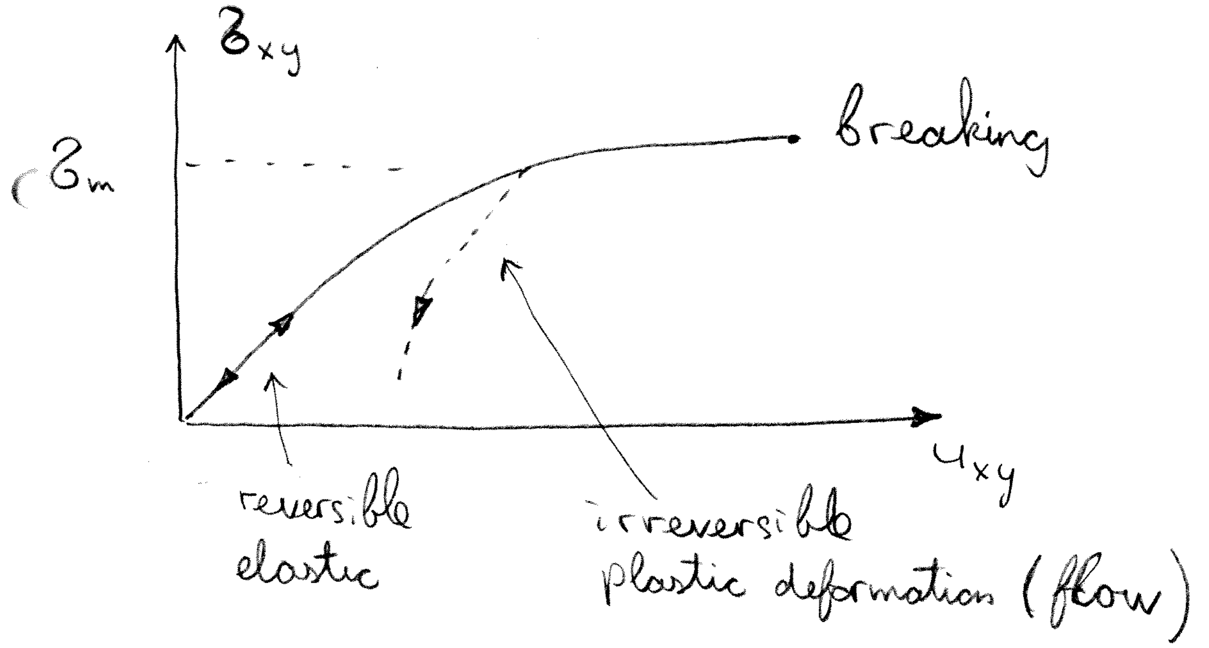
Dislocations

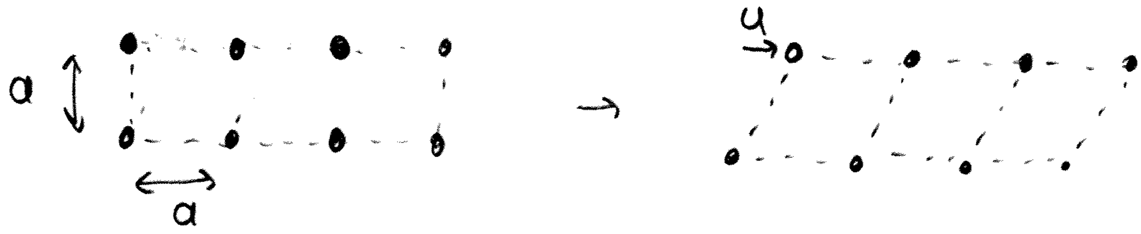
Hooke's law is linear response law.

With increase of deformation stress-strain relation becomes nonlinear



Let us estimate the <u>yield stress</u> 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 period a crystals goes to undeformed state.

It is natural to assume that the stress σ is 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

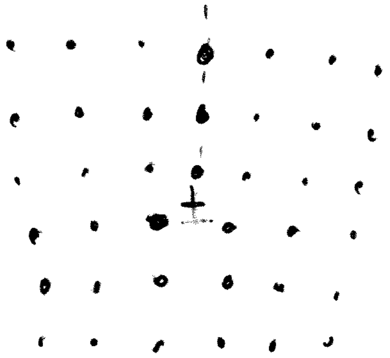
$$\sigma_m = \frac{\mu}{2\pi} \simeq \frac{\mu}{10}$$

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

Why ?

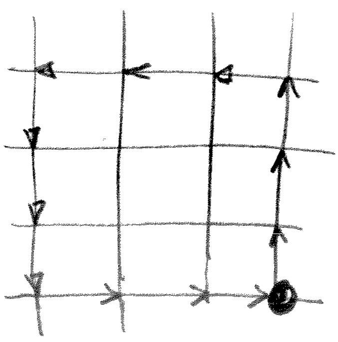
This is due to special defects called <u>dislocations</u>.

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

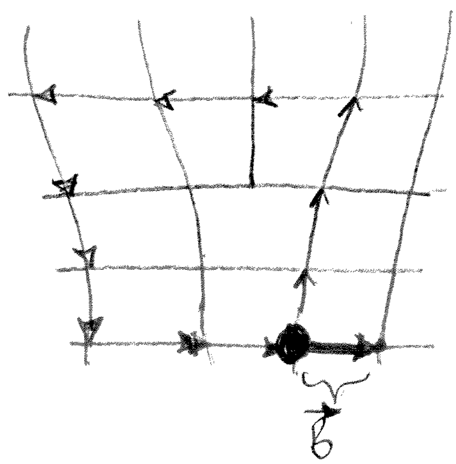


One can define it in the following way

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

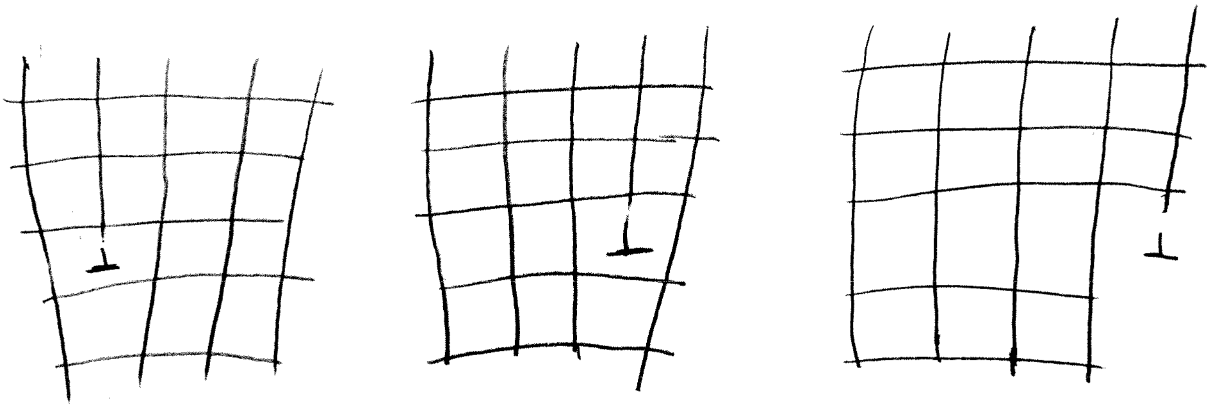


The same sequence of steps around dislocation will lead to displacement $\vec{b}$



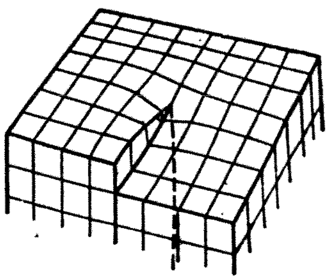
This vector $\vec{b}$ is called Burgers vector

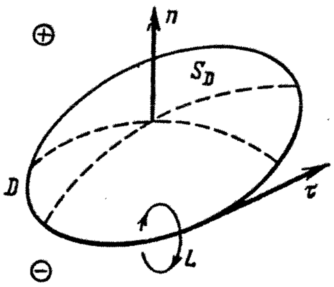
The Burgers vector doesn't depend on the chosen path => dislocation is topological defect. Although far away from its core deformations are small, by going around we can see that defect is present.

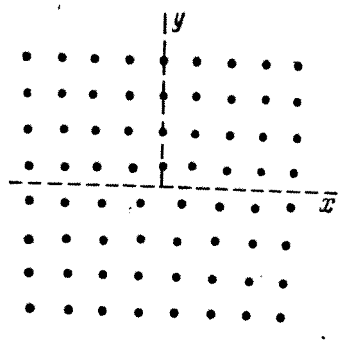


If dislocation moves through the crystal it produces shift of the upper half crystal by the unit vector $\vec{b}$. The shear that leads to the dislocation motion is much smaller than μ. That is why $\sigma_m << \mu$

Dislocations







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

$\vec{b}$ is called Burgers vector

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.

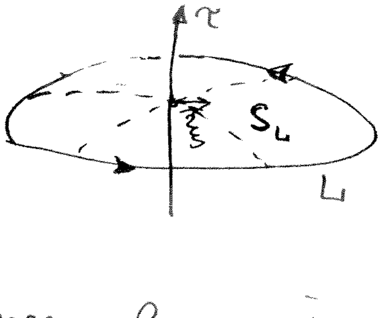
It is useful to introduce distorsion tensor

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

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

Eq. (1) (p. 79) 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 $\frac{\partial w_{mk}}{\partial x_l} = \frac{\partial^2 u_k}{\partial x_l \partial x_m}$

is symmetric $e_{ilm}\frac{\partial w_{mk}}{\partial x_l} \equiv 0$ 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

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

or

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

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

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

which can be rewritten through w_{ik}

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

Substituting condition (2) we obtain

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

$\Downarrow$

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

Screen 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 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 the form

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

(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

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

$$\vec{w} = \frac{1}{k^2}\left(\vec{f} - \frac{\vec{k}\cdot(\vec{k}\cdot\vec{f})}{k^2}\frac{1}{2(1-\sigma)}\right) \Rightarrow$$ (see p. 57)

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

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) p. 79 we can define $\vec{u}$ as continuous function on a plane with cut surface S_e: $\vec{u}_+ - \vec{u}_-\Big|_{S_e} = \vec{b}$. Then $F = \frac{1}{2}\int d^2r\, \sigma_{ij}u_{ij} = \frac{1}{2}\int d^2r\, \sigma_{ij}\nabla_j u_i =$

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