Recap:

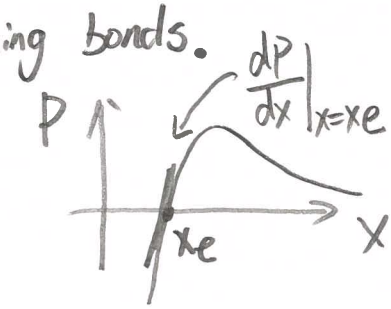
Notes on 04/18

* Three common crystal structures

BCC, FCC, HCP

* Elastic deformation is related to stretching bonds.

$$E = \frac{x_e}{A} \left.\frac{dP}{dx}\right|_{x=x_e}$$



* Theoretical Strength

$$\tau_b = \frac{Gb}{2\pi h} \approx \frac{G}{10},$$

τ_b is a few orders of magnitude higher than the actually measured strength, $\Rightarrow$ because of dislocation.

* Dislocation is 1-D defect

✓ edge dislocation, screw dislocation

✓ Burgers vector, measures distortion associated with a dislocation.

* plastic deformation is corresponding to dislocation motion.

* plastic strain and dislocation movement

dislocation density

$$\epsilon = b\rho\bar{x}$$

plastic strain

Burgers vector

average displacement of dislocation.

$$\boxed{\dot{\epsilon} = b\dot{\rho}\bar{x} + b\rho\bar{v}}$$

Orowan's equation

Notes on 04/18 (Thursday)

Dislocation : stress field and energy

The atoms in a crystal containing a dislocation are displaced from their perfect lattice sites, and the resulting distortion produces a stress field in the crystal around a dislocation.

Elasticity Theory :

The displacement of a point in a strained body from its position in unstrained state is writen as

$$\bar{u} = [u_x, u_y, u_z]$$

The components u_x, u_y, u_z represent projections of $\bar{u}$ on the x, y, z axes.

In linear elasticity, the nine components of strain are given in terms of the first derivatives of the displacement components :

$$e_{xx} = \frac{\partial u_x}{\partial x} \qquad e_{yy} = \frac{\partial u_y}{\partial y} \qquad e_{zz} = \frac{\partial u_z}{\partial z}$$

$$e_{xy} = e_{yx} = \frac{1}{2}\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right),$$

e.g. length l_x of an element in the x direction is changed to $l_x(1+e_{xx})$.

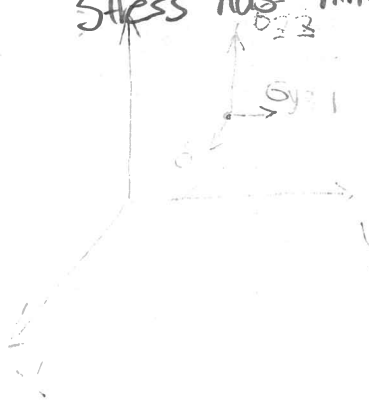
The volume V of a small volume element is changed by strain to

$$V+\Delta V = V(1+e_{xx})(1+e_{yy})(1+e_{zz})$$

$$\Rightarrow \Delta V/V = (1+e_{xx})(1+e_{yy})(1+e_{zz}) - 1, \qquad e_{xx}e_{yy} \ll e_{xx}/e_{yy}$$

$$\Rightarrow \Delta V/V = e_{xx} + e_{yy} + e_{zz}$$

Stress has nine components



σ_{xx} σ_{yy} σ_{zz} ← Normal stress

$$\boxed{\sigma_{xy} = \sigma_{yx}, \quad \sigma_{xz} = \sigma_{zx}, \quad \sigma_{yz} = \sigma_{zy}}$$ ← shear stress

↑ Due to rotational equilibrium

For linear isotropic solids:

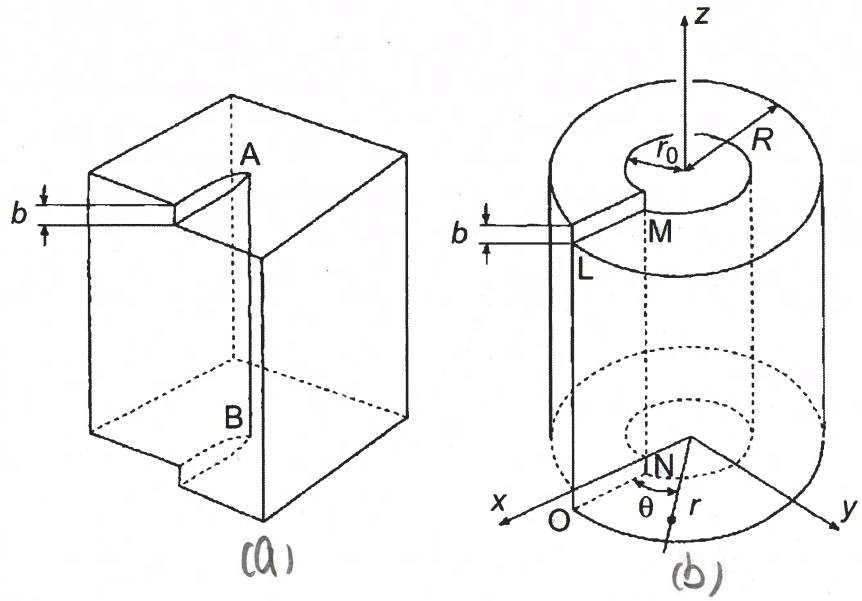
$$\sigma_{xx} = 2G e_{xx} + \lambda(e_{xx} + e_{yy} + e_{zz})$$

$$\sigma_{yy} = 2G e_{yy} + \;\vdots\;\vdots\;\vdots\;\vdots\;\vdots$$

$$\sigma_{zz} = 2G e_{zz} + \;\vdots\;\vdots\;\vdots\;\vdots\;\vdots$$

$$\sigma_{xy} = 2G e_{xy}, \quad \sigma_{yz} = 2G e_{yz}, \quad \sigma_{zx} = 2G e_{zx}$$

Stress field around screw dislocation



Consider the screw dislocation AB shown in (a); the elastic cylinder in (b) has been deformed to produce a similar distortion. A radial slit LMNO was cut in the cylinder parallel to the z-axis and the cut surface displaced rigidly with respect to each other by the distance b, the magnitude of the Burgers vector.

The elastic field in the dislocated cylinder can be found:

① there is NO displacement in the x and y directions.

$$u_x = u_y = 0$$

② the displacement in the z-direction increases uniformaly from 0 to b as θ increases from 0 to 2π:

$$u_z = \frac{b\theta}{2\pi} = \frac{b}{2\pi}\tan^{-1}(y/x)$$

the strain field is:

$$e_{xx} = e_{yy} = e_{zz} = e_{xy} = e_{yx} = 0$$

$$e_{xz} = e_{zx} = \frac{1}{2}\frac{\partial u_z}{\partial x} = -\frac{b}{4\pi}\frac{y}{(x^2+y^2)} = -\frac{b}{4\pi}\frac{\sin\theta}{r}$$

$$\left[\frac{b}{2\pi}\frac{\partial}{\partial x}\tan^{-1}(y/x) = \frac{b}{2\pi}\frac{1}{1+\frac{y^2}{x^2}}\frac{-y}{x^2} = \frac{-b}{2\pi}\frac{y}{x^2+y^2}\right]$$

$$e_{yz} = e_{zy} = \frac{b}{4\pi}\frac{x}{x^2+y^2} = \frac{b}{4\pi}\frac{\cos\theta}{r}$$

The components of stress are

$$\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = \sigma_{xy} = \sigma_{yx} = 0$$

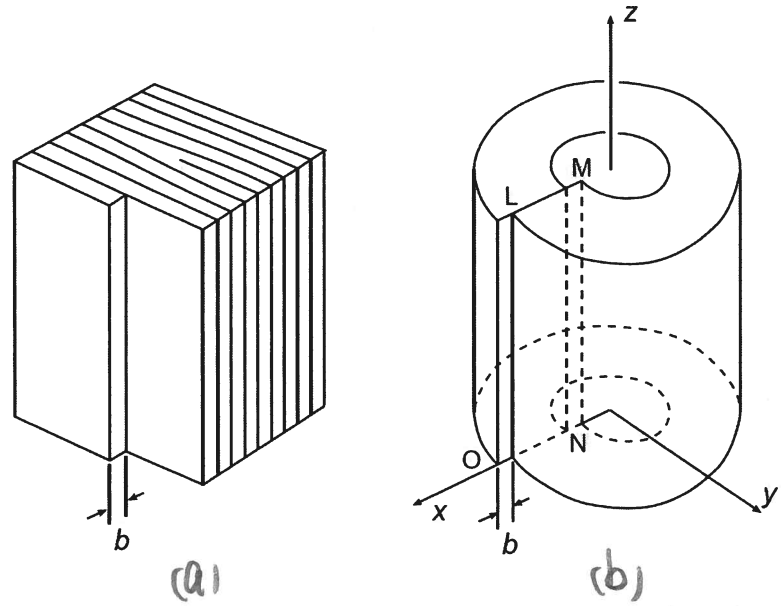
$$\sigma_{xz} = \sigma_{zx} = -\frac{Gb}{2\pi}\frac{r}{(x^2+y^2)} = -\frac{Gb}{2\pi}\frac{\sin\theta}{r}$$

$$\sigma_{yz} = \sigma_{zy} = \frac{Gb}{2\pi}\frac{x}{x^2+y^2} = \frac{Gb}{2\pi}\frac{\cos\theta}{r}$$

* the elastic distortion contains no tension or compression, and only consists of pure shear.

* the stress and strain are proportional to $1/r$, and therefor diverge to infinity as $r \to 0$. Elasticity theory breaks down, atomistic model must be used.

Stress field around edge dislocation



Considering the edge dislocation in the above figue. The displacement and strains in the z-direction are zero and the deformation is called plane strain. The stress can be found as.

$$\sigma_{xx} = -Dy\frac{3x^2+y^2}{(x^2+y^2)^2} \qquad \sigma_{yy} = Dy\frac{x^2-y^2}{(x^2+y^2)^2}$$

$$\sigma_{xy} = \sigma_{yx} = Dx\frac{x^2-y^2}{(x^2+y^2)^2} \qquad \sigma_{zz} = \nu(\sigma_{xx}+\sigma_{yy})$$

$$\sigma_{xz} = \sigma_{yz} = 0$$

where $D = \dfrac{Gb}{2\pi(1-\nu)}$

For edge dislocation:

* Displacement & strain in the z-direction are 0.
* plane strain deformation.

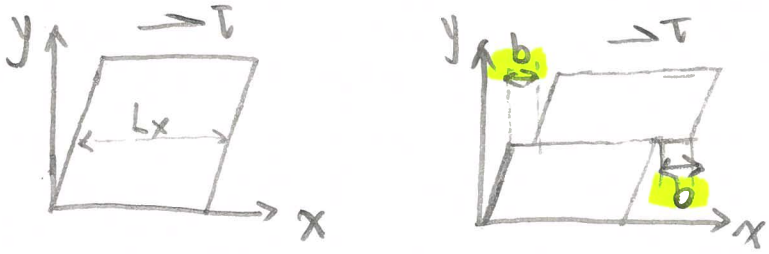
Force on Dislocations

Lecture Notes
04/23/2019 Tuesday

When a sufficiently high stress is applied to a crystal containing dislocations, the dislocations move and produce plastic strain. The load producing the applied stress therefore does work on the crystal when a dislocation moves, and so the dislocation responds to the stress as though it experiences a force equal to the work done divided by the distance it moves.

The force defined in this way is a virtual, rather than real, force.

Consider dislocation motion in a sample with dimension $L_x \times L_y \times L_z$ due to the shear stress τ:



The work done by the shear stress τ in changing the system is equal to

$$\tau \underset{\text{area}}{S} b = \tau L_x L_z b$$

If we consider the process as movement of a dislocation under the action of force F acting on a unit length of the dislocation, the same

work can also be written as

$$\underbrace{F \cdot L_z}_{} \times L_x$$

$$\Rightarrow \boxed{F = \tau b}$$

* The force acting on a dislocation line is Not a physical force, but a way to describe the tendency of dislocation to move through the crystal when stresses are present.

* The work done at the slip plane is dissipated into heat. (Similar to work done by friction forces)

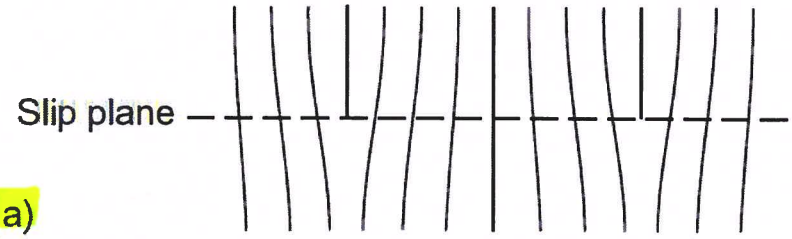
* τ is the shear stress in the glide plane resolved in the direction of $\hat{b}$, and $\hat{F}$ acts normal to the dislocation line.

Since the dislocation moves on its glide plane, we only need to consider the shear stress on this plane.

Moreover, only shear stress components in the direction of $\hat{b}$ are contributed to the movements of the dislocation.

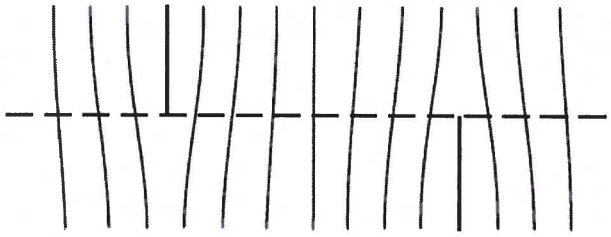
Forces between Dislocations

like dislocations on the same slip plane →



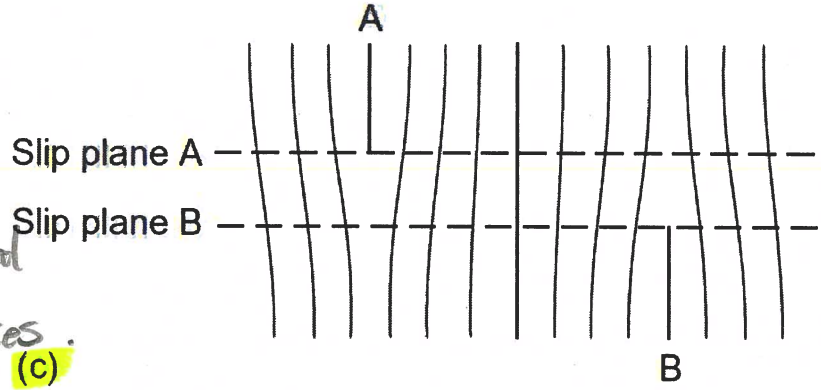
(a)

unlike dislocations on the same slip plane



(b)

unlike dislocations on slip planes seperated by a few atomic spaces.



(c)

Elastic energy associated with a dislocation is (per unit length)

$$E_{el} = \alpha G b^2$$

$\alpha \approx 0.5 \sim 1.0$.

(a) Consider two parallel edge dislocations lying in the same slip plane.

They have the same sign [above figure (a)]

when they are seperated by a large distance, the total elastic

energy per unit length will be

$$\alpha G b^2 + \alpha G b^2 = 2\alpha G b^2$$

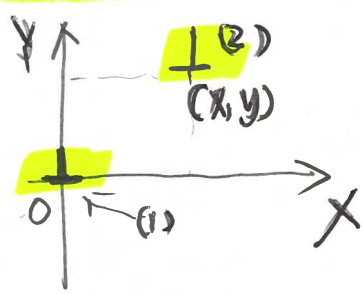
When they are very close together, it becomes a single dislocation with Burgers vector magnitude $2b$, and elastic energy will be given by

$$\alpha G (2b)^2 = 4\alpha G b^2$$

energy is twice of the seperated dislocation with large distance.

Thus the dislocations will tend to repel each other to reduce their total elastic energy.

(b) when two opposite sign dislocations of are close together, the Burgers vector magnitude becomes 0. Thus the dislocations will attract each other to reduce their total energy. In figure (b), the two will combine and annihilate each other.



(c)

In general, the force acting on dislocation is given as

$$F_x = \frac{Gb^2}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2}$$ ← in the glide direction

$$F_y = \frac{Gb^2}{2\pi(1-\nu)} \frac{y(3x^2-y^2)}{(x^2+y^2)^2}$$ ← perpendicular to the glide plane.

If two dislocations have the same sign,

(1) $y < x < \infty$, $F_x > 0$, repulsive

(2) $y = x$, $F_x = 0$, unstable

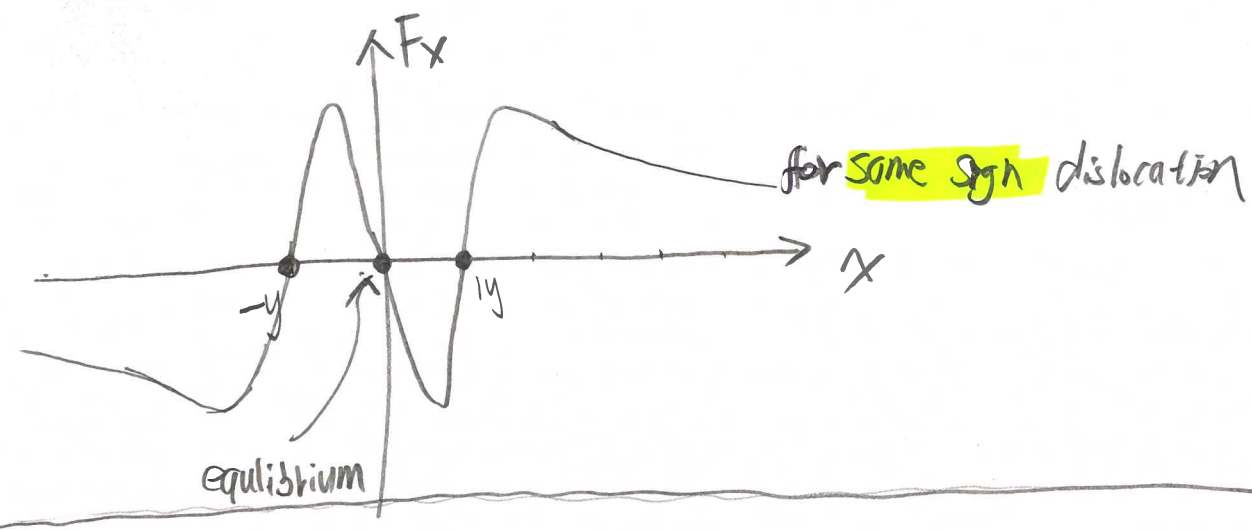
(3) $0 < x < y$, $F_x < 0$, attractive

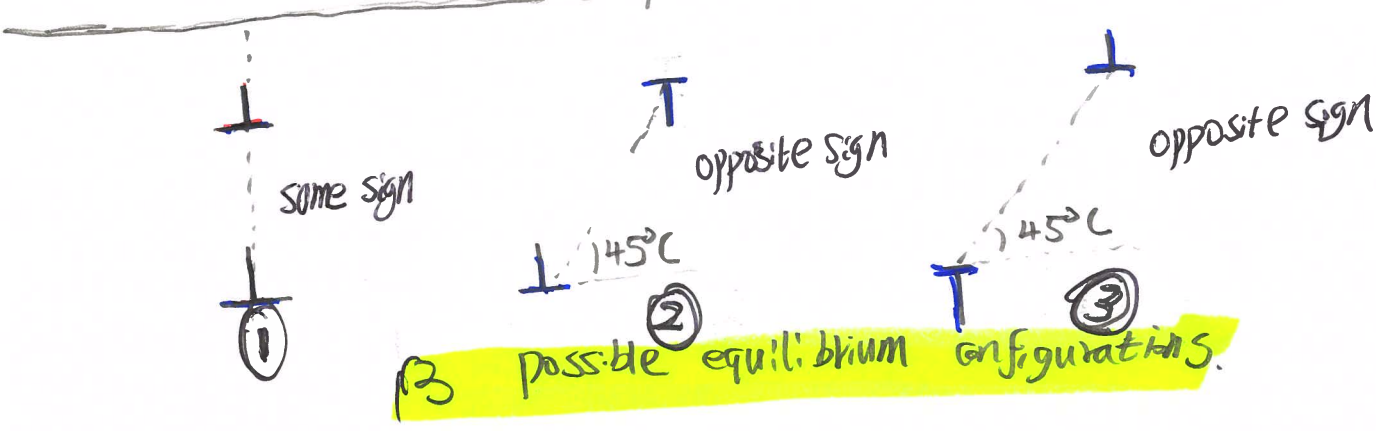
(4) $x = 0$, $F_x = 0$, equlibrium

(5) $-y < x < 0$ $F_x > 0$, attractive

(6) $x = -y$ $F_x = 0$, unstable

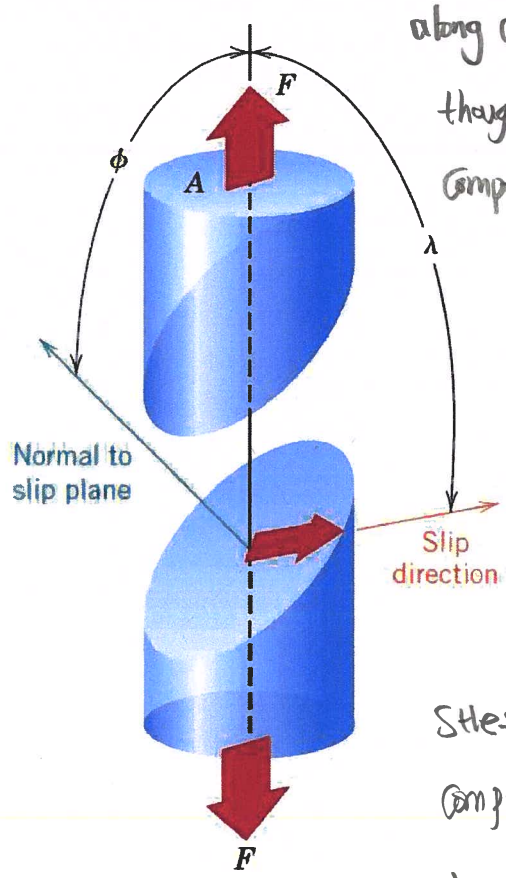
(7) $-\infty < x < -y$ $F_x < 0$, repulsive.





3 possible equilibrium configurations.

Resolved Shear Stress



Dislocations moves in response to shear stress applied along a slip plane and in a slip direction. Even though an applied stress may be pure tensile, shear components exist in other directions.

Consider the crystal in the left figure, which is being deformed in tension by an applied force F along the cylindrical axis.

If the crossectional area is A, the tensile stress parallel to F is $\sigma = F/A$. The force has a component $F \cdot \cos\lambda$ in the slip direction, where λ is the angle between F and the slip direction.

The force acts over the slip surface which has an area $A/\cos\phi$, where ϕ is the angle between F and the normal to the slip plane.

Thus the shear stress τ, resolved on the slip plane in the slip direction is

$$\boxed{\tau = \frac{F}{A}\cos\phi\cos\lambda = \sigma\cos\phi\cos\lambda}$$

* in general: $\phi + \lambda \neq 90$, because the tensile axis, the slip plane normal, and the slip direction do not always lie in the same plane.

Critical Resolved shear Stress (CRSS)

τ_{CRSS} – the minimum shear stress required to begin plastic deformation deformation or slip.

* Depending on material, temperature, strain rate

* the system on which slip occurs has the largest $\boxed{\cos\phi \cos\lambda}$

Schmid factor

* $(\cos\phi \cos\lambda)_{max} = \cos 45^\circ \cos 45^\circ = \frac{1}{2}$

$\tau_{max} = \sigma/2$, τ_{CRSS}

when $\tau_{max} > \tau_{CRSS}$ $\Longrightarrow$ plastic deformation

i.e. $\frac{\sigma}{2} > \tau_{CRSS}$

$\Rightarrow \boxed{\sigma > 2\tau_{CRSS}}$

Recap

Notes on 4/25/2019

* Stress field around screw dislocation

$$\sigma_{xz} = \sigma_{zx} = -\frac{Gb}{2\pi}\frac{\sin\theta}{r}$$

$$\sigma_{yz} = \sigma_{zy} = \frac{Gb}{2\pi}\frac{\cos\theta}{r}$$

* Stress field around edge dislocation

$$\sigma_{xz} = \sigma_{zx} = \sigma_{yz} = \sigma_{zy} = 0$$

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

$$\sigma_{xy} = \sigma_{yx} = Dx\frac{x^2-y^2}{x^2+y^2}, \quad D = \frac{Gb}{2\pi(1-\nu)}$$

* Force on Dislocation (per length)

$$\underbrace{\tau L_x L_z}\, b = \underbrace{F \cdot L_z}\, \times \underbrace{L_x}_{\text{glide distance}}$$

$$\Rightarrow \boxed{F = \tau b}$$

* Energy associated with a dislocation

$$E_{el} = \alpha G b^2 \propto b^2$$

* Force between Dislocation

(a)

same sign, the same slip plane, Repulsive

$x \to \infty$, $E_\infty = \alpha G b^2 + \alpha G b^2 = 2\alpha G b^2$

$x = 0$, $E_0 = \alpha G (2b)^2 = 4\alpha G b^2$

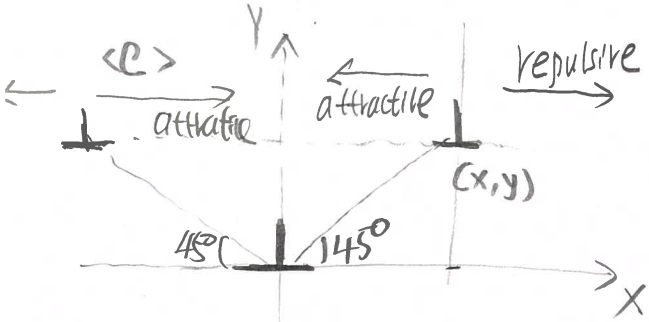
(b)

opposite sign, the same slip plane, Attractive

$x \to \infty$, $E_\infty = 2\alpha G b^2$

$x = 0$, $E_0 = 0$

(c)



$$F_x = \frac{G b_1 b_2}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2}$$

x range	Fx	nature
$-\infty < x < -y$	<0	repulsive
$-y < x < 0$	>0	attractive
$0 < x < y$	<0	attractive
$y < x < \infty$	>0	repulsive

$\Downarrow$ equilibrium position

<(C)>

dislocation dipoles.

$$F_x = \frac{G b_1 b_2}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2},$$ b_1 b_2 have opposite sign.

* Resolved Shear Stress

$$\tau = \sigma \cos\phi \cos\lambda$$

$\frac{F}{A}$

angle between F and the slip direction

angle between F and the normal to the slip plane

* Critical Resolved Shear Stress τ_{CRSS}

$\sigma > 2\tau_{CRSS}$ for plastic deformation.

e.g. A metal single crystal is oriented with the [101] parallel to the tensile stress axis. If the slip plane is (111) and slip direction is $\frac{a}{2}[1\bar{1}0]$, calculate the stress necessary to activate slip if the critical resolved shear stress is 0.34 MPa.

stress axis [101]

slip plane normal [111]

slip direction $[1\bar{1}0]$, $\tau = \sigma \cos\phi \cos\lambda$

$$\cos\phi = \frac{[101][111]}{|[101]||[111]|} = \frac{2}{\sqrt{2}\sqrt{3}} = \sqrt{\frac{2}{3}}$$

$$\cos\lambda = \frac{[101][1\bar{1}0]}{|[101]||[1\bar{1}0]|} = \frac{1}{\sqrt{2}\times\sqrt{2}} = \frac{1}{2}$$

$$\tau = \sigma \cdot \sqrt{\frac{2}{3}}\,\frac{1}{2} = \sigma\sqrt{\frac{1}{6}}$$

if $\tau > \tau_{CRSS}$, slip starts.

i.e. $\sigma\sqrt{\frac{1}{6}} > 0.34$ MPa

$\Rightarrow \sigma = 0.34 \times \sqrt{6}$ MPa

$\simeq 0.83$ MPa

Lecture #9

Work-hardening in polycrystals / single crystals

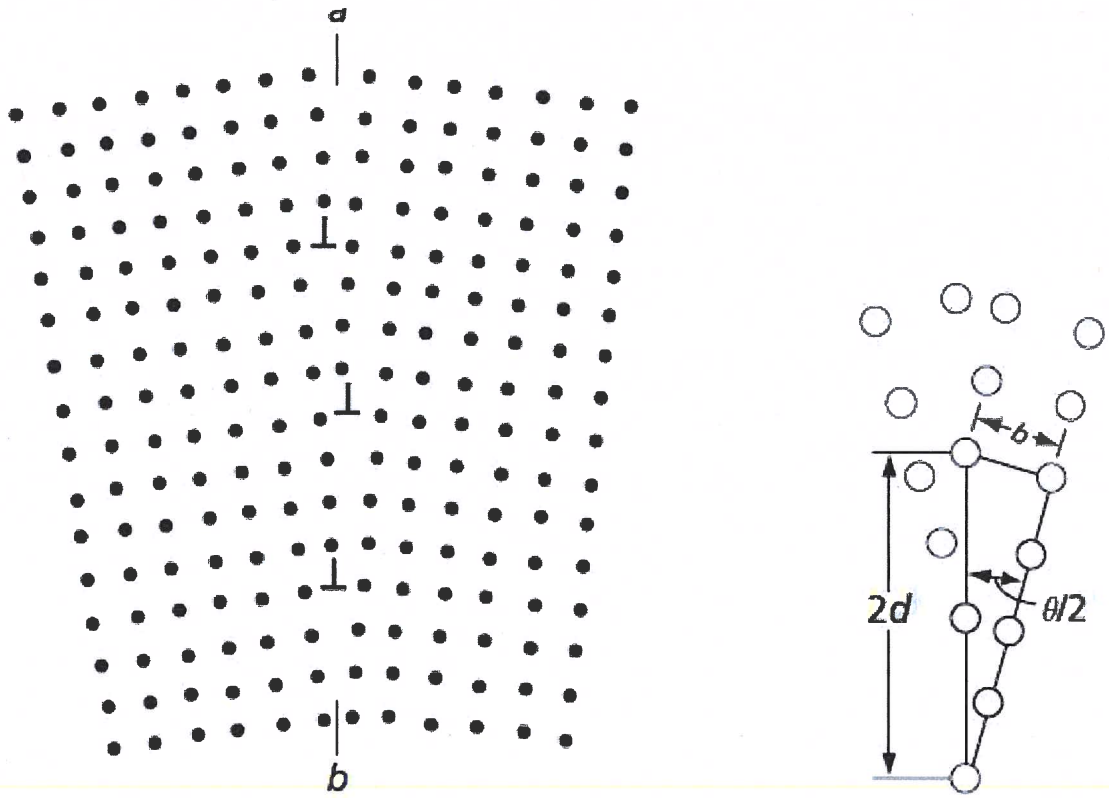
The plastic deformation increases the dislocation density. The relationship between the flow stress and the dislocation density is

$$\tau = \tau_0 + \alpha G b \rho^{1/2}$$

where α is a constant with a value between 0.3 ~ 0.6. τ_0 is the stress necessary to move a dislocation in the absence of other dislocations.

Low angle grain boundary

two grains differ only slightly in their relative orientation.



(A) (B)

Dislocation model of small angle grain boundary.

The geometrical relation-ship between θ, the angle of tilt, and d the spacing between the dislocations is

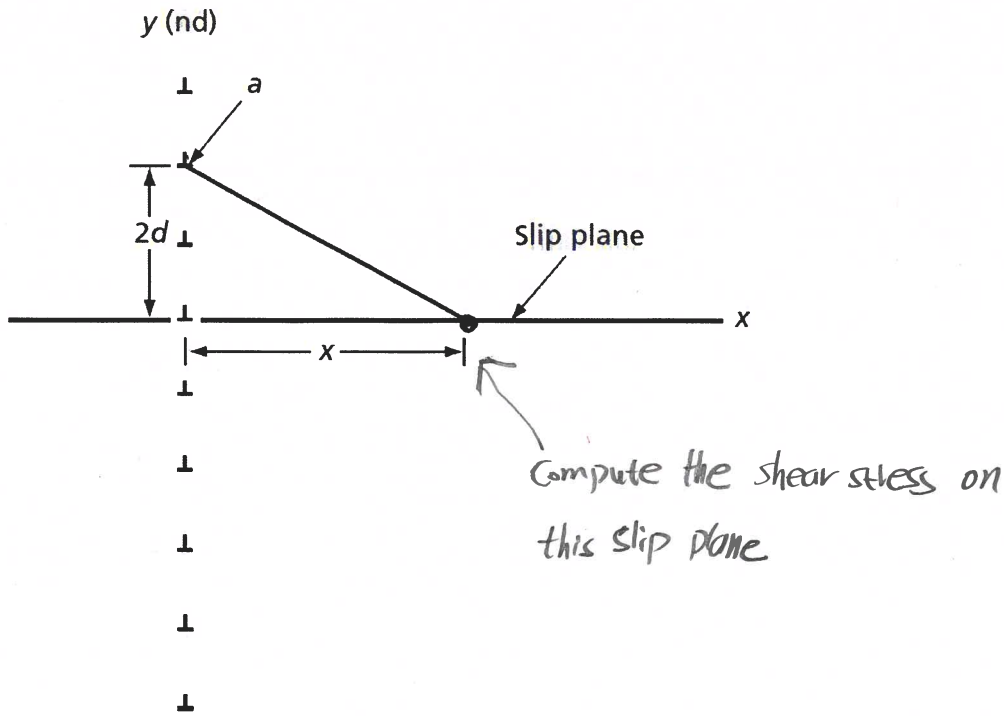
$$\sin\frac{\theta}{2} = \frac{b}{2d}$$

, b is the Burgers vector, d is spacing between the dislocations.

if θ is very small, $\sin\frac{\theta}{2} \simeq \frac{\theta}{2}$

$$\Rightarrow \theta = b/d$$

Stress field of a grain boundary



The shear stress around an edge dislocation is:

$$\sigma_{xy} = Dx\frac{x^2-y^2}{(x^2+y^2)^2}, \quad D = \frac{Gb}{2\pi(1-\nu)}$$

The positions of dislocation is $y = nd$, where d is dantance between dislocation distance, and n is dislocation number.

For dislocation at point a, i.e. $n=2$,

$$\sigma_{xy} = D\frac{x(x^2-4d^2)}{(x^2+4d^2)^2}$$

Summing the stress from all the dislocations, we obtain

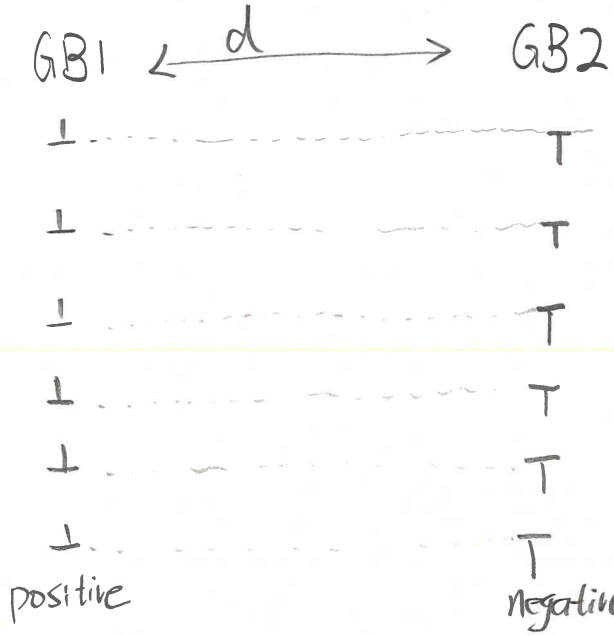
$$\sigma_{xy} = D\sum_{n=-\infty}^{n=\infty}\frac{x(x^2-(nd)^2)}{(x^2+(nd)^2)^2}$$

$$\Rightarrow \sigma_{xy} = D\frac{\pi^2 x}{d^2(\sinh^2(\pi x/d))}$$

collection!!

hyperbolic function

Energy of grain boundary (GB)



two infinitly long parallel tilt boundaries

$d \to \infty$, $E_{total} = E_{GB1} + E_{GB2}$

$d \to 0$, $E_{total} = 0$.

Force attracting the dislocation toward each other is $\sigma_{xy} b$

The energy per length requiral to seperate the two boundary equals

$$W = \int_0^\infty \sigma_{xy} b \, dx$$

$$= \int_0^\infty D\frac{\pi x \, b}{d^2(\sinh^2(\pi x/d))} dx$$

$$\boxed{E = \frac{1}{2} W = \frac{Gb}{4\pi(1-\nu)} \theta (A - \ln \theta)}$$ energy per area.

Variation of GB energy with misorientation (see slides)

Grain boundary in plastic deformation

Hall and Petch equation.

$$\sigma_y = \sigma_0 + k D^{-1/2}$$

σ_y is the yield stress;

σ_0 is a frictional stress required to move dislocations;

k is H-P slop;

D is grain size.

- **HW2 is due at 9:30AM. If you want to obtain solutions for the problems, submit yours to Canvas or email them to me, and I will send you a copy of the solutions.**

- **Midterm exam will be given in class at 9:30 AM Tuesday, 05/07/2019.**

- **Tips on preparing exam - reviewing slides and lecture notes, and finishing HW2.**