Module #13

Elastic Properties of Dislocations

Stacking faults

READING LIST

DIETER: Ch. 5, Pages 160-168

Ch. 4, Pages 205-222 in Meyers & Chawla, 1st ed.

Introduction

- Dislocations are line defects that distort the perfect crystal lattice.

- This lattice distortion produces an elastic stress field inside the crystal.

► The magnitude of the elastic stress field can be estimated using elasticity theory. The next viewgraph provides a general explanation of why.

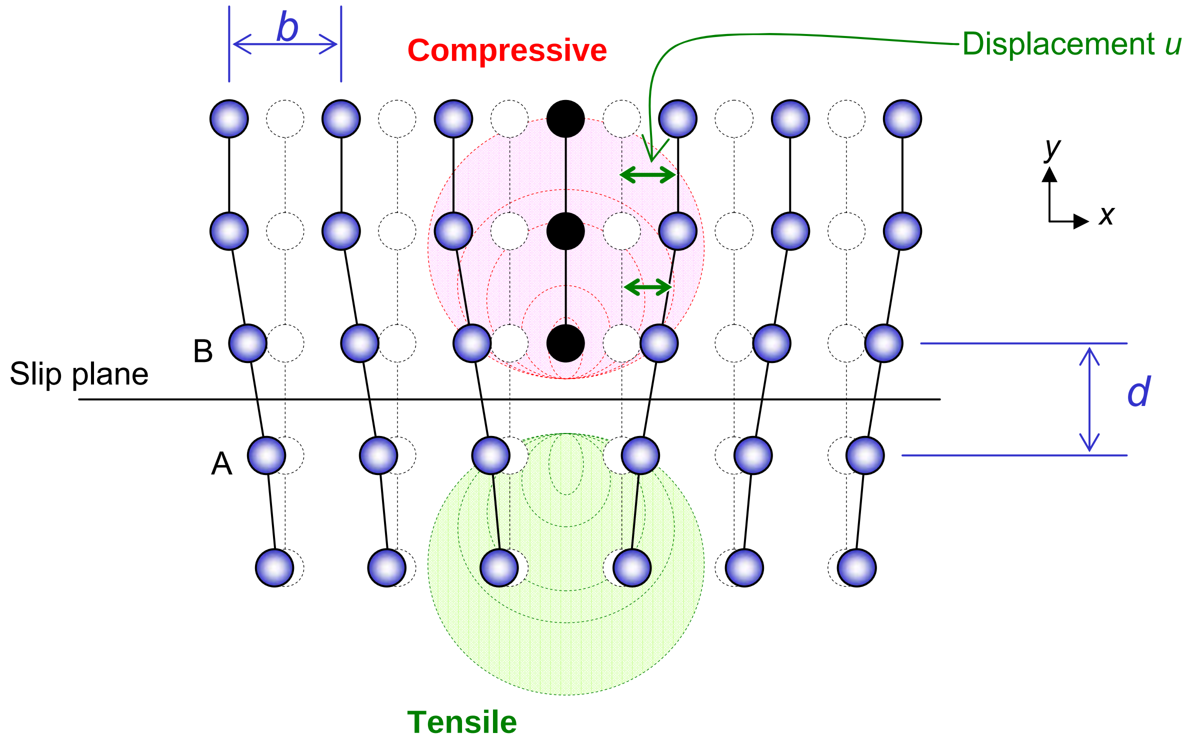
► We can in turn use this information to determine the energy of the dislocation, the force it exerts on other dislocations, and its energy of interaction with other defects.

- Interactions between the stress fields (i.e., the distorted regions) around dislocations (and those of other defects) ultimately determine the mechanical properties of the lattice.

Strain energy of a dislocation

- The energy of a dislocation comes from the distortion associated with the displacement of atoms from their equilibrium positions.

- Near the center of the dislocation (i.e., along the dislocation line), the displacements are too large to be calculated with elasticity theory. Hooke's law does not apply here. This region is called the *dislocation core*.



★ *A few lattice spacings from the core*, say at a distance r_o, *we can model things using elasticity theory as the displacements are very small*. Hooke's law applies here. r_o is called the *cutoff radius*. It typically has a value near b.

Strain Energy

- Strain increases the internal energy of a body. The elastic strain energy per unit volume is given by:

$$\frac{\text{Elastic strain energy}}{\text{Volume}} = \frac{1}{2} \sum_{i=x,y,z} \sum_{j=x,y,z} \sigma_{ij} e_{ij}$$

- Thus, for an element of volume *dV*, the elastic strain energy can be expressed as:

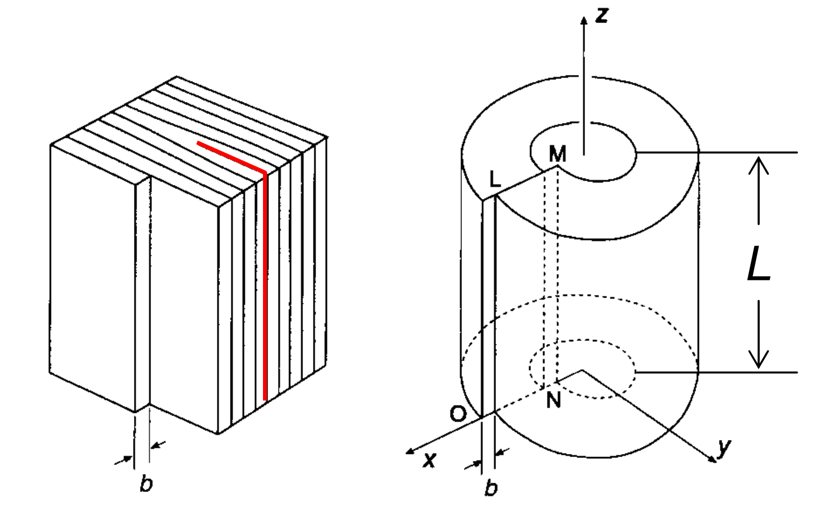
$$dE_{\text{elastic}} = \frac{1}{2} dV \sum_{i=x,y,z} \sum_{j=x,y,z} \sigma_{ij} e_{ij}$$

- We can utilize this expression to estimate the elastic strain energy for a dislocation by incorporating the components of stress and strain that surround the dislocation.

- A crystal containing a dislocation is not at its lowest energy state. There is a *strain energy* term (E_{total}) that must be added to the lattice energy of the crystal.

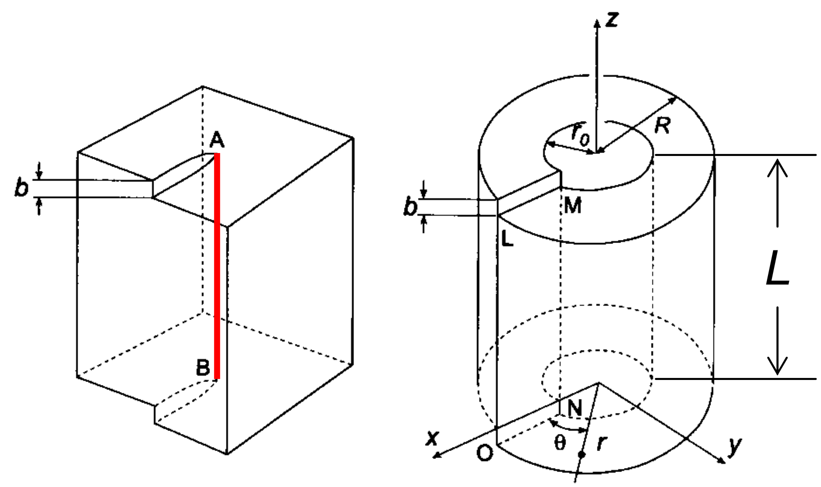
- The distortions caused by the presence of edge and screw dislocations are simulated on cylindrical diagrams to the right. The diagrams depict each type of dislocation as a distorted cylinder.

- Using these diagrams, we can calculate the strain energy on the basis of elasticity theory. This is detailed in Hull and Bacon [1] and in Weertman and Weertman [2].



(a) (b) [Hull and Bacon]

Figure 4.6 (a) Edge dislocation formed in a crystal. (b) Elastic distortion of a cylindrical ring simulating the distortion produced by the edge dislocation in (a).



(a) (b) [Hull and Bacon]

Figure 4.5 (a) Screw dislocation *AB* formed in a crystal. (b) Elastic distortion of a cylindrical ring simulating the distortion produced by the screw dislocation in (a).

[1] D. Hull and D.J. Bacon, Introduction to Dislocations, 4th ed. (Butterworth-Heinemann, Oxford, 2001), pp.62-72.
[2] J. Weertman and J.R. Weertman, Elementary Dislocation Theory (Oxford University Press, Oxford, 1992), pp. 32-40,

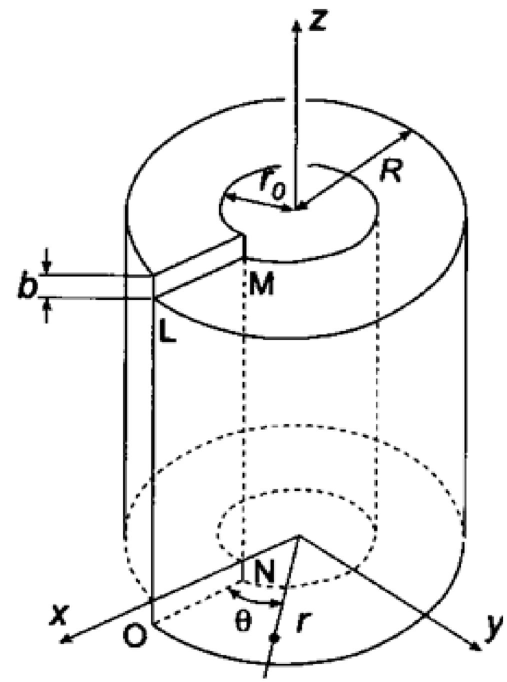
Screw Dislocation

- Elastic stresses around a screw dislocation:

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

$$\tau_{yz} = \tau_{zy} = \frac{Gb}{2\pi}\frac{x}{\left(x^2+y^2\right)} = \frac{Gb}{2\pi}\frac{\cos\theta}{r}$$

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



[Hull and Bacon]

- All shear components parallel to the dislocation line.

Edge Dislocation

- Elastic stresses around an edge dislocation:

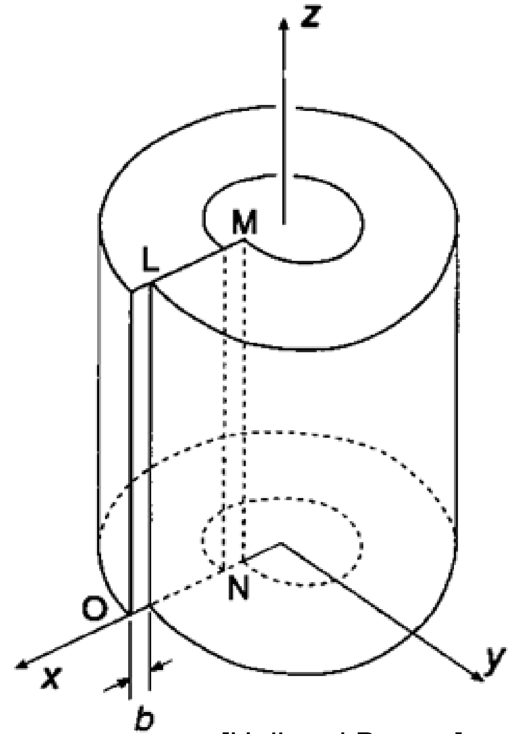
$$\sigma_{xx} = -\frac{Gb}{2\pi(1-\nu)} \frac{y(3x^2+y^2)}{(x^2+y^2)^2}$$

$$\sigma_{yy} = \frac{Gb}{2\pi(1-\nu)} \frac{y(x^2-y^2)}{(x^2+y^2)^2}$$

$$\tau_{xy} = \tau_{yx} = \frac{Gb}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2}$$

$$\sigma_{zz} = \nu(\sigma_{xx}+\sigma_{yy}) = -\frac{Gb\nu}{\pi(1-\nu)} \frac{y}{x^2+y^2}$$

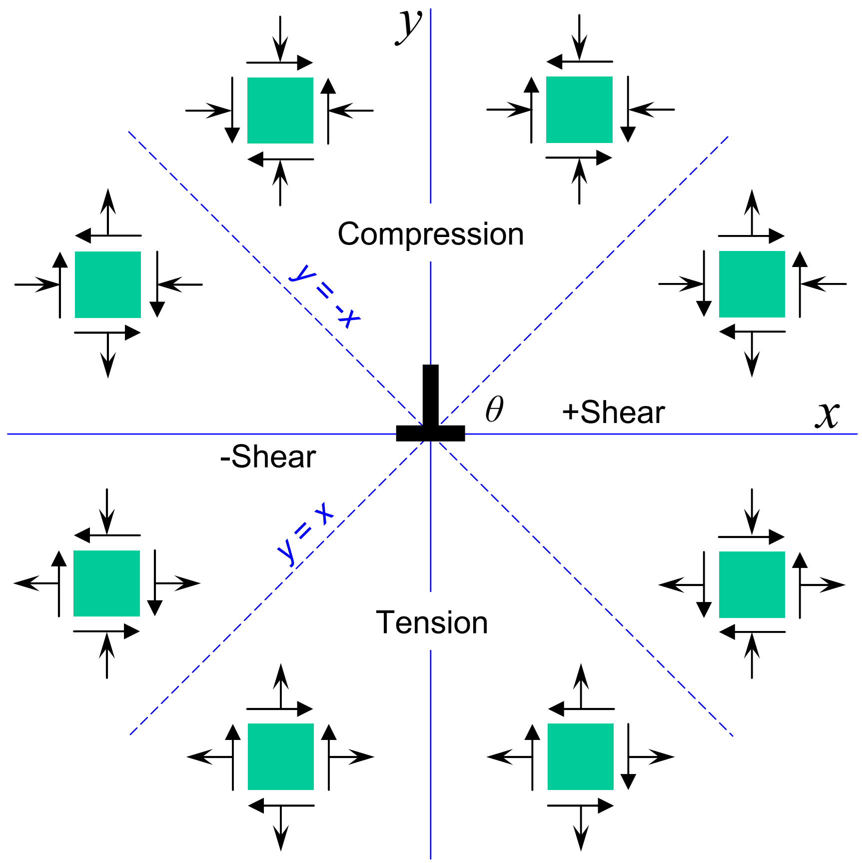
$$\tau_{xz} = \tau_{zx} = \tau_{yz} = \tau_{zy} = 0$$



[Hull and Bacon]

- Stress field has dilatational and shear components.

Stress fields around an edge dislocation



Schematic representation of the stress field about an edge dislocation

- E_{total} can be divided into two parts:

$$E_{\text{total}} = E_{\text{core}} + E_{\text{elastic (strain energy)}}.$$

- The core contribution (E_{core}) is difficult to calculate. It is estimated to have a value of ≈0.5 eV/plane threaded by a dislocation.

- From elasticity theory, the *elastic strain energy per unit length of dislocation* is given by:

$$E_{\text{elastic}}^{\text{SCREW}} = \frac{Gb^2}{4\pi}\int_{r_o}^{R}\frac{dr}{r} = \frac{Gb^2}{4\pi}\int_{r_o}^{R}\frac{dx}{x} = \frac{Gb^2}{4\pi}\ln\left(\frac{R}{r_o}\right) \qquad \therefore \boxed{E_{\text{elastic}}^{\text{SCREW}} \propto Gb^2}$$

$$E_{\text{elastic}}^{\text{EDGE}} = \frac{Gb^2}{4\pi(1-\nu)}\int_{r_o}^{R}\frac{dx}{x} = \frac{Gb^2}{4\pi(1-\nu)}\ln\left(\frac{R}{r_o}\right) \qquad \therefore \boxed{E_{\text{elastic}}^{\text{EDGE}} \propto \frac{Gb^2}{(1-\nu)} \cong 1.5Gb^2}$$

$$E_{\text{elastic}}^{\text{MIXED}} = \left[\frac{Gb^2\sin^2\theta}{4\pi(1-\nu)} + \frac{Gb^2\cos^2\theta}{4\pi}\right]\ln\left(\frac{R}{r_o}\right)$$

- For all of the different types of dislocations, the value of E_{elastic} depends on r_o and the crystal radius R through a slowly varying logarithmic term. This is illustrated in the figure on the next page.

Elastic strain energy per unit length of dislocation

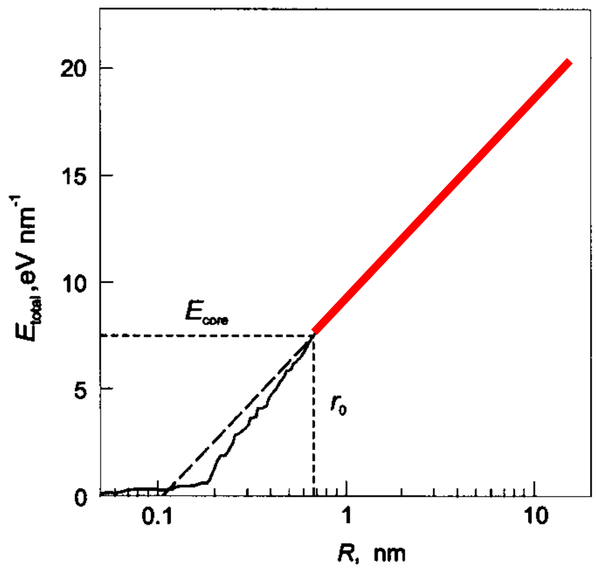


Figure 4.7 The strain energy within a cylinder of radius R that contains a straight edge dislocation along its axis. The data was obtained by computer simulation for a model of iron. (Courtesy Yu. N. Osetsky.)

[Hull & Bacon]

- The value of E_{elastic} depends weakly on r_o and the crystal radius R through a slowly varying logarithmic term *outside of the core region*.
- We can approximate E_{elastic} for any type of dislocation as:

$$\boxed{E_{\text{elastic}} = \alpha G b^2}$$

where $\alpha \approx 0.5 - 1.0$

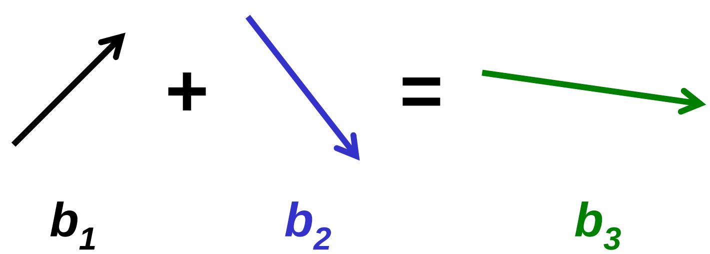
$$OR$$

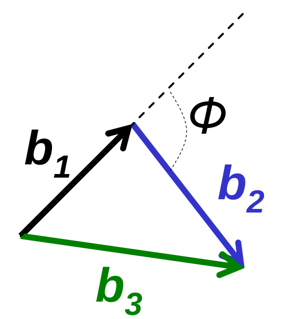
$$E_{\text{elastic}} \propto b^2$$

$$E_{\text{elastic}}(screw) < E_{\text{elastic}}(edge) < E_{\text{elastic}}(mixed)$$

$$E_{\text{elastic}} = \alpha G b^2$$
$$\text{where } \alpha \approx 0.5 - 1.0$$

- One of the important consequences of this relationship is that it <u>allows for determination</u> of <u>whether or not</u> it is energetically feasible for two <u>dislocations</u> to <u>react/combine to form another</u>.
- This is generally known as <u>*Frank's Rule*</u>.





$\boldsymbol{b_1} + \boldsymbol{b_2} = \boldsymbol{b_3}$

IMPORTANT
Elastic strain energy $\propto Gb^2$

Yes if $\left(b_1^2 + b_2^2\right) > b_3^2$

No if $\left(b_1^2 + b_2^2\right) < b_3^2$

No net energy change if $\left(b_1^2 + b_2^2\right) = b_3^2$

Dislocations of unit strength

- The Burgers vector of a crystal must also connect one equilibrium lattice position to another.

- Crystal structure determines Burgers vector.

►If Burgers vector = one lattice spacing then the dislocation is of unit strength.

Dissociation of dislocations

- Because of energy considerations it is possible for some dislocations with strengths greater than or equal to unity to dissociate (split) into shorter segments.

Will the reaction $b_1 \rightarrow b_2 + b_3$ occur?

Yes if $b_1^2 > \left(b_2^2 + b_3^2\right)$

No if $b_1^2 < \left(b_2^2 + b_3^2\right)$

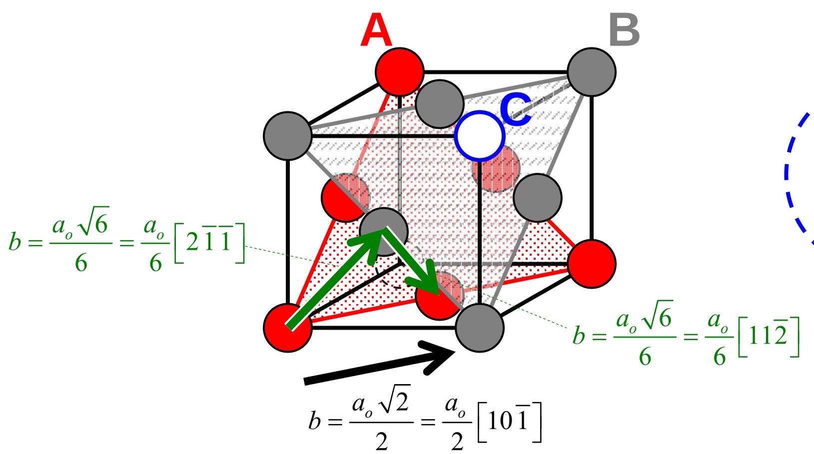
IMPORTANT
Elastic strain energy $\propto Gb^2$

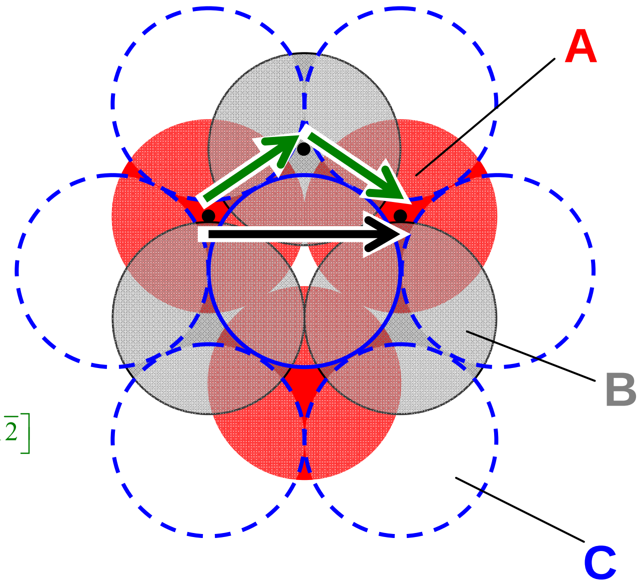
- This is occurs in some *close-packed* (i.e., FCC and HCP) *crystals* such as where equilibrium positions are not the edges of the unit cell.

- Can have serious implications on plastic deformation.

Dissociation of a unit dislocation in an FCC crystal

- In this example, the separation into partial dislocations is energetically favorable. There is a decrease in strain energy.





Reaction $b_1 \rightarrow b_2 + b_3$ will occur if $b_1^2 > \left(b_2^2 + b_3^2\right)$

$$\frac{a_o}{2}\left[10\bar{1}\right] \rightarrow \frac{a_o}{6}\left[2\bar{1}\bar{1}\right] + \frac{a_o}{6}\left[11\bar{2}\right]$$

$$\frac{a_o^2}{2} > \frac{a_o^2}{6} + \frac{a_o^2}{6}$$

- The separation produces a *stacking fault* between the partials.

Forces on dislocations

- When the stresses applied to a crystal are large enough, dislocations will move resulting in plastic deformation. Deformation will occur via slip or climb.

- The applied load induces work on the crystal during dislocation motion.

- In turn, the dislocation responds to the applied stress as though it were experiencing a force. The force is given by:

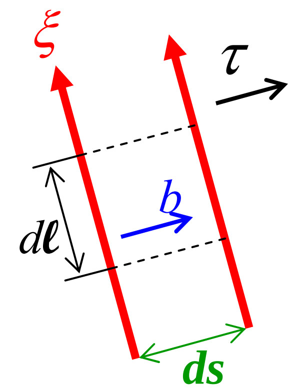
$$F = \frac{\text{Work req'd. to move } \perp}{\text{Distance moved}}$$

We will consider the glide/slip force now and the climb force later.

Glide force on a dislocation

- If we consider a glissile dislocation (ξ) under an applied shear stress (τ). The dislocation has a Burgers vector b.

- When a segment of the dislocation line $d\ell$ moves forward a distance ds, the regions of the crystal above and below the slip plane are displaced relative to each other by a distance that is equivalent to the Burgers vector, b.



Displacement ds of an element $d\ell$ in its slip plane used to determine the glide force.

- The average shear displacement of the crystal due to glide of segment $d\ell$ is thus:

$$dx = \left(\frac{ds\, d\ell}{A} \right) b$$

- where A is the area of the entire slip plane.

Forces on dislocations (2)

- The external force (f) acting uniformly on this small area (due to τ) is:

$$f = A\tau$$

- The work done when the small element $d\boldsymbol{\ell}$ glides forward is therefore:

$$dW = \text{force} \times \text{displacement} = f dx = (A\tau)\left[\left(\frac{ds\, d\ell}{A}\right)b\right] = \tau(ds\, d\ell)b = \tau b dA$$

- Since force = work divided by the distance over which it is applied (ds), the glide force per unit length on a dislocation ($d\boldsymbol{\ell}$), F_L, is:

$$F_L = \frac{f}{d\ell} = \frac{dW/ds}{d\ell} = \frac{dW}{dA} = \tau b$$

τ is the shear stress in the slip plane resolved in the direction of b.

- This force, which is the result of externally applied stress, acts normal to the dislocation line along its length. This is the Peach-Koehler equation. It is often given as:

$$\boldsymbol{F} = F_L d\ell = (\sigma \cdot b) \times d\ell = (\sigma \cdot b) \times \xi$$

A more advanced treatment is provided in the following five pages

General Peach-Koehler equation

- Most dislocations are mixed. Mixed dislocations are oriented such that the tangent to the dislocation line (i.e., the sense vector ξ, $\hat{t}$, or $\boldsymbol{\ell}$) is neither parallel or perpendicular to the Burgers vector. In this case:

$$b = b_x i + b_y j + b_z k$$

- In 3D space, all will have components parallel to the *x,y,z* axes. We also need to account for components of stress that are parallel to the *x,y,z* axes.

- If we let $g = \sigma_{ij} \cdot b$, then:

$$\begin{aligned} g_x &= b_x \sigma_{xx} + b_y \tau_{xy} + b_z \tau_{xz} \\ g_y &= b_x \tau_{yx} + b_y \sigma_{yy} + b_z \tau_{yz} \\ g_z &= b_x \tau_{zx} + b_y \tau_{zy} + b_z \sigma_{zz} \end{aligned}$$

and

$$F_L = g \times \xi = \begin{vmatrix} i & j & k \\ g_x & g_y & g_z \\ \xi_x & \xi_y & \xi_z \end{vmatrix}$$

where F_L is the force per unit length of dislocation. This is essentially *F/L* for a straight dislocation where *L* is the length of the dislocation line.

This general form of the Peach-Koehler equation is used to calculate the magnitudes of the forces on and the forces between dislocations.

B*

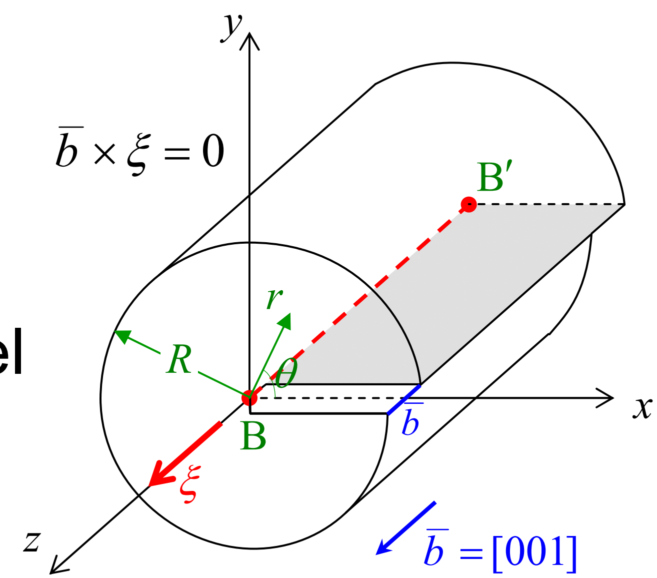
Forces exerted on a straight **screw** dislocation

- Elastic stresses around a screw dislocation:

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

$$\tau_{yz} = \tau_{zy} = \frac{Gb}{2\pi}\frac{x}{\left(x^2+y^2\right)} = \frac{Gb}{2\pi}\frac{\cos\theta}{r}$$

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



- All shear components acting parallel to the dislocation line.

- Thus:

$$\sigma_{screw} = \begin{vmatrix} 0 & 0 & \tau_{xz} \\ 0 & 0 & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & 0 \end{vmatrix} = \begin{vmatrix} 0 & 0 & \tau_{xz} \\ 0 & 0 & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & 0 \end{vmatrix}$$

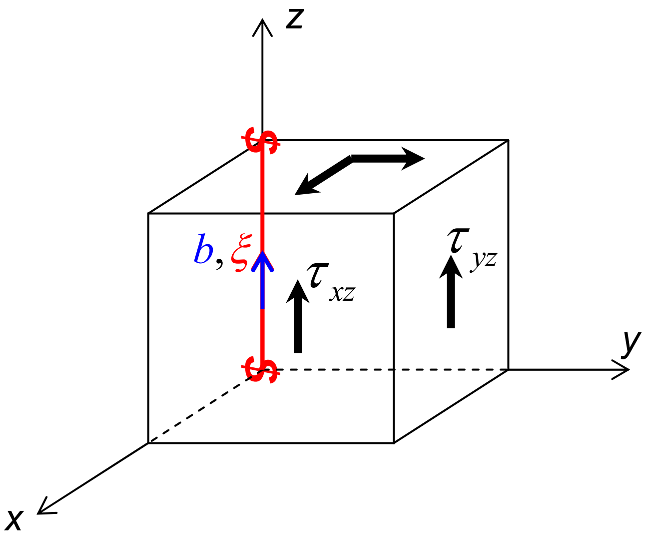
and

$$g_x = \tau_{xz} b$$
$$g_y = \tau_{yz} b$$
$$g_z = 0$$

B*

General Peach-Koehler equation – cont'd

- Consider a straight **screw dislocation** as illustrated below.



- For this screw dislocation: $b = [001]$ and $\xi = [001]$. Therefore,

$$(\sigma \cdot b) = b \begin{vmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} \end{vmatrix} \begin{vmatrix} 0 \\ 0 \\ 1 \end{vmatrix}$$

$$= b \begin{vmatrix} \tau_{xz} & \tau_{yz} & \sigma_{zz} \end{vmatrix}$$

- Taking the cross product of $(\sigma \cdot b)$ and the line sense (ξ) we get:

$$F_L = (\sigma \cdot b) \times \xi = \begin{vmatrix} i & j & k \\ b\tau_{xz} & b\tau_{yz} & b\sigma_{zz} \\ 0 & 0 & 1 \end{vmatrix} = b\tau_{yz} i - b\tau_{xz} j = F_x + F_y$$

NOTE: This also proves that two shear stresses act upon this screw dislocation.

This tells us that only τ_{xz}, and τ_{yz} can exert a force on this dislocation and that the force acts perpendicular to the dislocation line along its length.

B*

Forces exerted on a straight **edge** dislocation

- Elastic stresses around an edge dislocation:

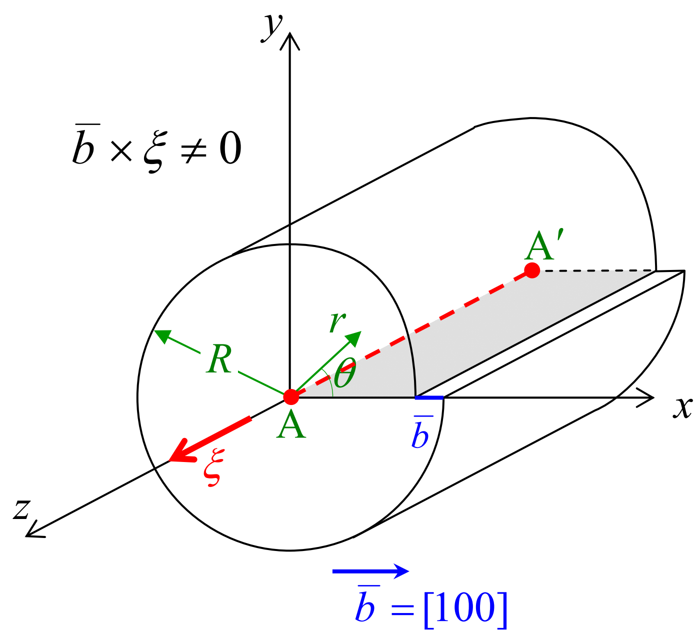
$$\sigma_{xx} = -\frac{Gb}{2\pi(1-\nu)}\frac{y\left(3x^2+y^2\right)}{\left(x^2+y^2\right)^2}$$

$$\sigma_{yy} = \frac{Gb}{2\pi(1-\nu)}\frac{y\left(x^2-y^2\right)}{\left(x^2+y^2\right)^2}$$

$$\tau_{xy} = \tau_{yx} = \frac{Gb}{2\pi(1-\nu)}\frac{x\left(x^2-y^2\right)}{\left(x^2+y^2\right)^2}$$

$$\sigma_{zz} = \nu\left(\sigma_{xx}+\sigma_{yy}\right) = -\frac{Gb\nu}{\pi(1-\nu)}\frac{y}{x^2+y^2}$$

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



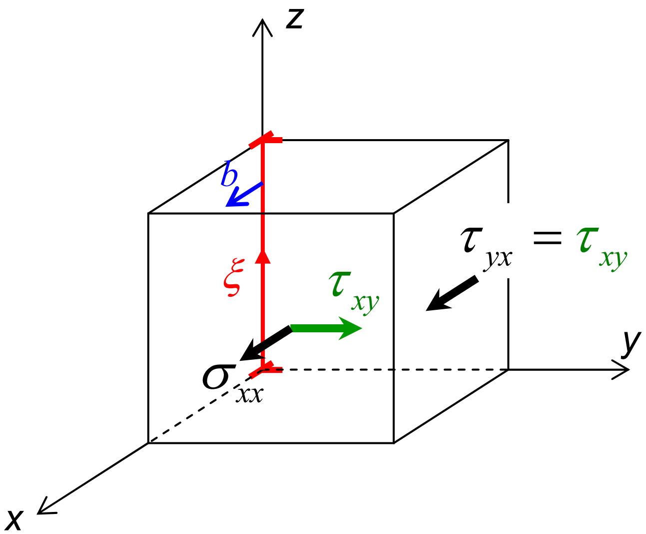
- Thus:

$$\sigma_{edge} = \begin{vmatrix} \sigma_{xx} & \tau_{xy} & 0 \\ \tau_{yx} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{vmatrix} = \begin{vmatrix} \sigma_{xx} & \tau_{xy} & 0 \\ \tau_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{vmatrix} \quad \text{and} \quad \begin{aligned} g_x &= \sigma_{xx} b \\ g_y &= \tau_{yz} b \\ g_z &= 0 \end{aligned}$$

B*

General Peach-Koehler equation – cont'd

- Consider a straight **edge dislocation** as illustrated below.



- For this edge dislocation: b = [100] and ξ = [001]. Therefore,

$$(\sigma \cdot b) = b \begin{vmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} \end{vmatrix} \begin{vmatrix} 1 \\ 0 \\ 0 \end{vmatrix}$$

$$= b \begin{vmatrix} \sigma_{xx} & \tau_{yx} & \tau_{zx} \end{vmatrix} = b \begin{vmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \end{vmatrix}$$

- Taking the cross product of ($\sigma \cdot b$) and the line sense (ξ) we get:

$$F_L = (\sigma \cdot b) \times \xi = \begin{vmatrix} i & j & k \\ b\sigma_{xx} & b\tau_{xy} & b\sigma_{xz} \\ 0 & 0 & 1 \end{vmatrix} = b\tau_{xy} i - b\sigma_{xx} j = F_x + F_y$$

NOTE: This also proves that one normal stress and one shear stress act upon this screw dislocation.

This tells us that only τ_{xy} and σ_{xx} can exert a force on this dislocation and that the force acts perpendicular to the dislocation line along its length. F_x is the glide force (+y direction). while F_y is the climb force (in –y direction).

B*

Bending of Dislocations - 1

- In addition to the Peach-Koehler force, dislocations develop a *line tension*.
- Line tension develops because the strain energy of a dislocation is proportional to its length.
- Any increase in length, increases the strain energy of the dislocation in proportion to its length.

Bending of Dislocations - 2

► Therefore, dislocations bend and/or always try to straighten out to reduce their lengths.

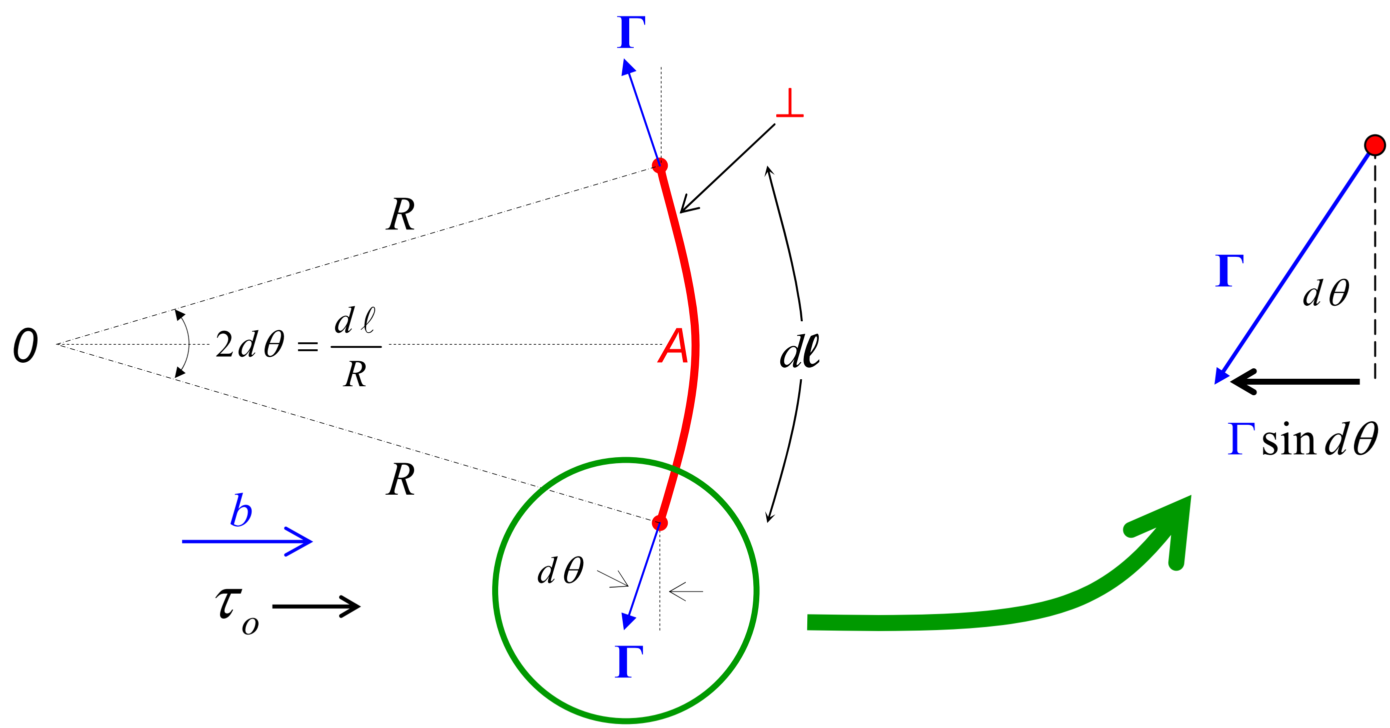
- Straight dislocations are shorter and thus have lower strain energies than curved dislocations.

- The line tension, Γ, which is the increase in energy per unit increase in dislocation length can be expressed as:

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

Line tension on dislocations (1)

- Consider the curved dislocation illustrated below.



- A specific shear stress, τ_o, is required to overcome Γ and maintain the radius of curvature, R.
- τ_o is maximum when $d\theta$ = 90°

Line tension on dislocations (2)

- The outward force (f_{out}) due to applied stress τ_o is:

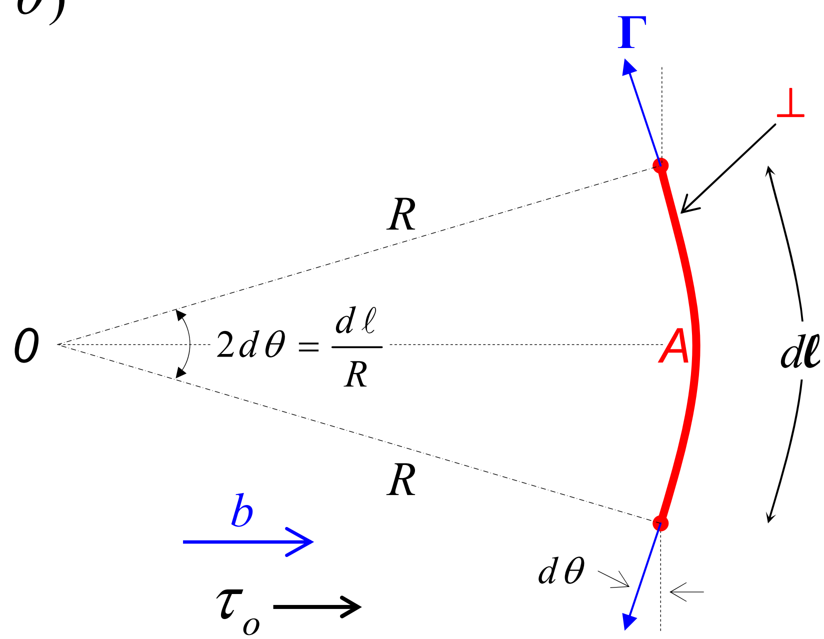
$$f_{out} = (\tau_o b)\, d\ell = 2\tau_o R d\theta$$ ← [Peach-Koehler equation ($F_L = \sigma b$)]

- The outward force is opposed by a line tension force acting along OA. It is given by:

$$f_{tension} = 2\Gamma \sin(d\theta)$$
$$= 2\Gamma d\theta \quad \text{(for small values of } \theta\text{)}$$

- Curvature will be maintained if:

$$f_{tension} = f_{out}$$
$$2\Gamma d\theta = 2\tau_o b R d\theta$$
$$\tau_o = \frac{\Gamma}{bR} = \frac{\alpha G b}{R}$$



Line tension on dislocations (3)

$$\tau_o = \frac{\alpha G b}{R}$$ [Stress required to bend $\perp$ to radius R]

- This equation provides an adequate approximation for most dislocations (it does, however, make some generally invalid assumptions).

- We will use a version of this when we discuss strengthening via the immobilization of dislocations.

- See Hirth and Lothe, Friedel, or another text on dislocations for more detailed treatment.

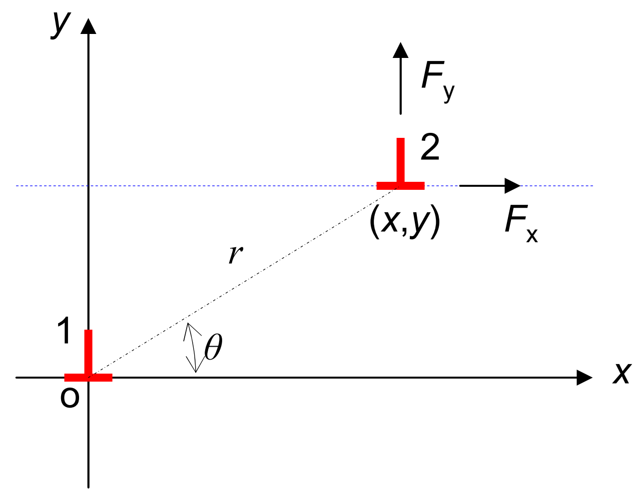
There is a significance to the concept of forces on dislocations.

★ Dislocations will <u>always</u> try to adopt configurations that will reduce their total elastic strain energies.

Interactions/forces between dislocations

Edge dislocations

- What is the force on dislocation 2 due to the presence of dislocation 1? The dislocations have parallel Burgers vectors.



- Parallel edge dislocations:

$$\xi = [001];\ b_1, b_2 = [100]$$

$$F_{1-2} = \begin{bmatrix} F_x \\ F_y \\ F_z \end{bmatrix} = (\sigma_1 \cdot b_2) \times \xi_2 = \left(\begin{bmatrix} \sigma_{xx} & \tau_{xy} & 0 \\ \tau_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{bmatrix} \bullet b_2 \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \right) \times \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \sigma_{xx} b_2 \\ \tau_{xy} b_2 \\ 0 \end{bmatrix} \times \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

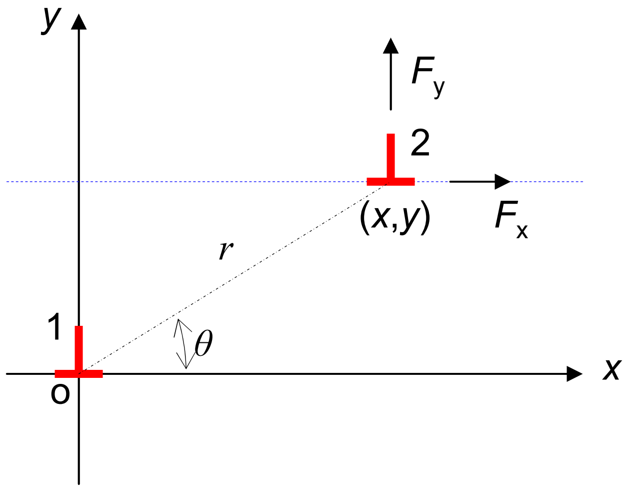
$$= \begin{vmatrix} i & j & k \\ \sigma_{xx} b_2 & \tau_{xy} b_2 & 0 \\ 0 & 0 & 1 \end{vmatrix} = (\tau_{xy} b_2) i - (\sigma_{xx} b_2) j$$

$$\therefore\ F_x = \tau_{xy} b_2 \quad \text{and} \quad F_y = -\sigma_{xx} b_2$$

B* [glide] [climb]

Forces between dislocations (4)

Edge dislocations



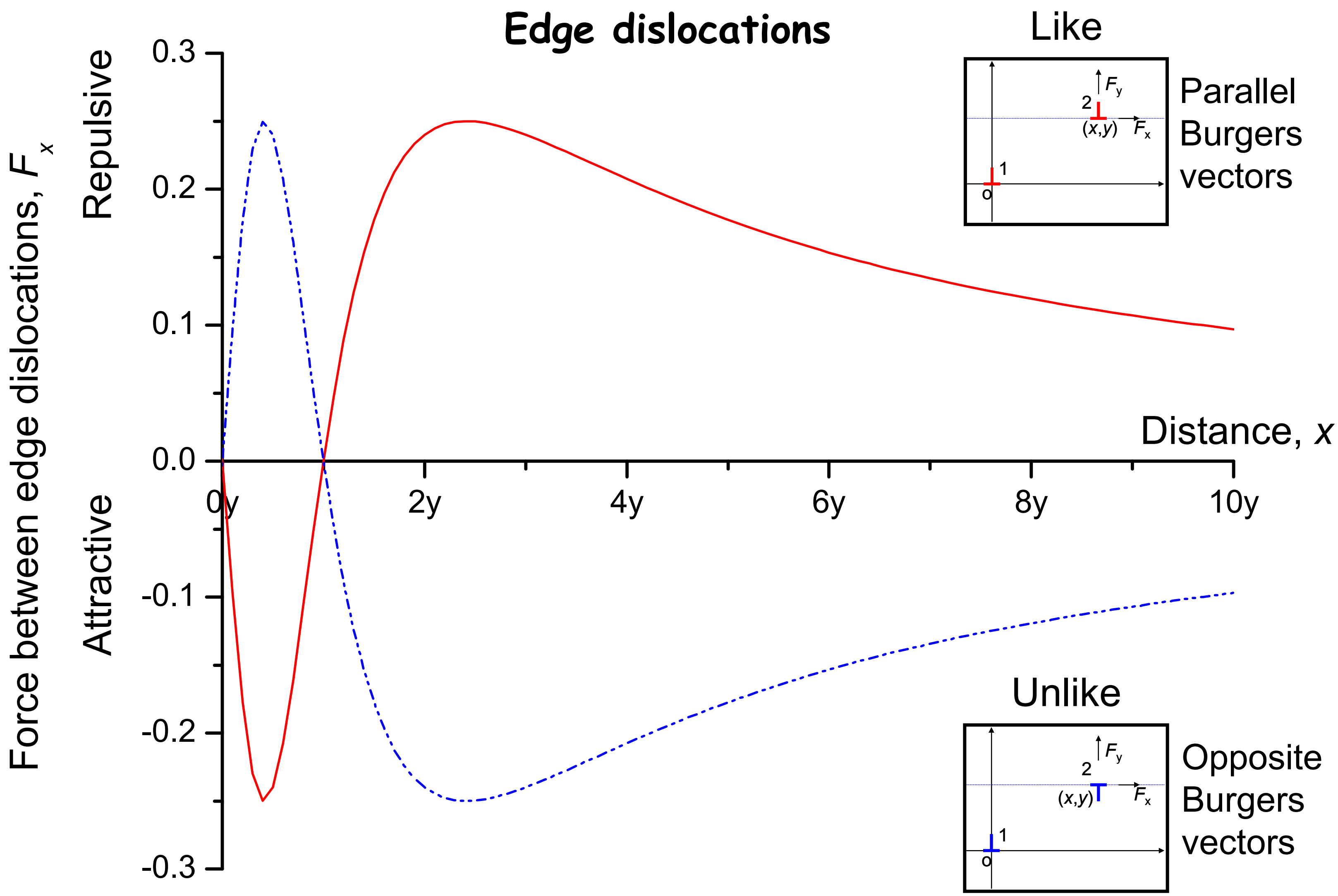
Glide force: $F_x = b_2\tau_{xy} = \dfrac{Gb_1b_2}{2\pi(1-\nu)}\dfrac{x(x^2-y^2)}{(x^2+y^2)^2}$

Climb force: $F_y = -b\sigma_{xx} = \dfrac{Gb_1b_2}{2\pi(1-\nu)}\dfrac{y(3x^2+y^2)}{(x^2+y^2)^2}$

General equation:
$$F = \frac{Gb_1b_2}{2\pi(1-\nu)r}\left[\cos\theta\left(\cos^2\theta-\sin^2\theta\right)i+\sin\theta\left(1+\cos^2\theta\right)j\right]$$
$$= \frac{Gb_1b_2}{2\pi(1-\nu)r}\left[\left(\cos\theta\cos2\theta\right)i-\sin\theta\left(2+\cos2\theta\right)j\right]$$
$$= \frac{Gb_1b_2}{2\pi(1-\nu)r}\left[F_x(\theta)+F_y(\theta)\right]$$

B*

Forces between dislocations (5)

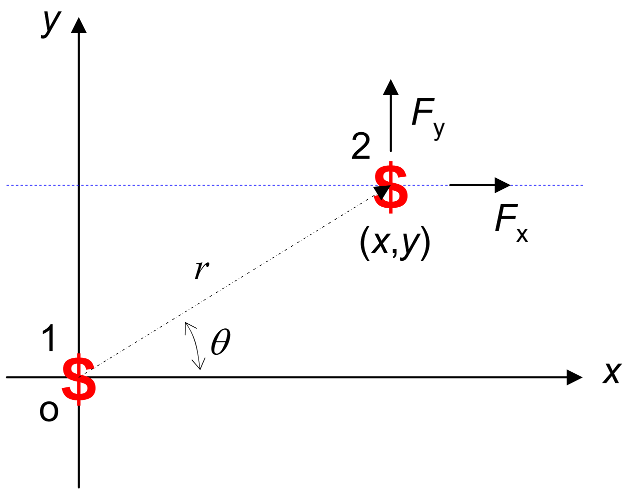


The implications of this distribution of stresses is that ***dislocations will assume different configurations depending upon their type, sign, and orientation***.

Interactions/forces between dislocations

Screw dislocations

- What is the force on dislocation 2 due to the presence of dislocation 1? The dislocations have parallel Burgers vectors.



- Parallel screw dislocations:

$$\xi = [001];\ b_1, b_2 = [100]$$

$$F_{1-2} = \begin{bmatrix} F_x \\ F_y \\ F_z \end{bmatrix} = (\sigma_1 \cdot b_2) \times \xi_2 = \left(\begin{bmatrix} 0 & 0 & \tau_{xz} \\ 0 & 0 & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & 0 \end{bmatrix} \bullet b_2 \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \right) \times \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \tau_{xz} b_2 \\ \tau_{yz} b_2 \\ 0 \end{bmatrix} \times \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

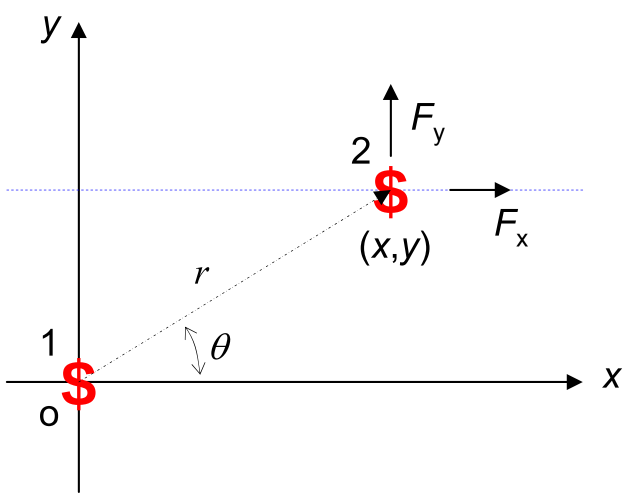
$$= \begin{vmatrix} i & j & k \\ \tau_{xz} b_2 & \tau_{yz} b_2 & 0 \\ 0 & 0 & 1 \end{vmatrix} = (\tau_{yz} b_2) i - (\tau_{xz} b_2) j$$

$$\therefore\ F_x = \tau_{yz} b_2 \quad \text{and} \quad F_y = -\tau_{xz} b_2$$

B*

Forces between dislocations (6)

Screw dislocations



Glide force: $F_x = b_2 \tau_{yz} = \dfrac{Gb_1b_2}{2\pi} \dfrac{x}{(x^2+y^2)} = \dfrac{Gb_1b_2}{2\pi r} \cos\theta$

Climb force: $F_y = -b_2 \tau_{yz} = \dfrac{Gb_1b_2}{2\pi} \dfrac{y}{(x^2+y^2)} = \dfrac{Gb_1b_2}{2\pi r} \sin\theta$

General equation: $F = \dfrac{Gb_1b_2}{2\pi r} \cos\theta i + \sin\theta j$

B*

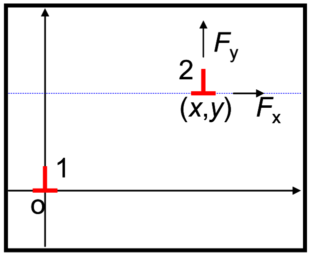
Climb Force

- The component F_y is a *mechanical climb force per unit length*.

- It results from the normal stress of dislocation #1 attempting to push the extra half plane of dislocation #2 from the crystal.

► This only occurs if point defects can be emitted from or absorbed by the core of dislocation #2.

► Creation and annihilation of point defects induces *chemical forces* due to changes in defect concentration.



$$\boxed{F_y = \frac{Gb^2}{2\pi(1-\upsilon)} \frac{y(3x^2+y^2)}{(x^2+y^2)^2}}$$

Mechanical Force

$$c = \exp\left[-\left(E_f^v + F\Omega/b\right)/kT\right]$$
$$= c_o \exp\left(-F\Omega/bkT\right)$$

where $\Omega =$ atomic volume,

$k =$ Boltzman's const.,

$T =$ temperature,

$c_o =$ equilibrium vacancy conc.

$$\boxed{f_y = \frac{bkT}{\Omega} \ln\left(\frac{c}{c_o}\right)}$$

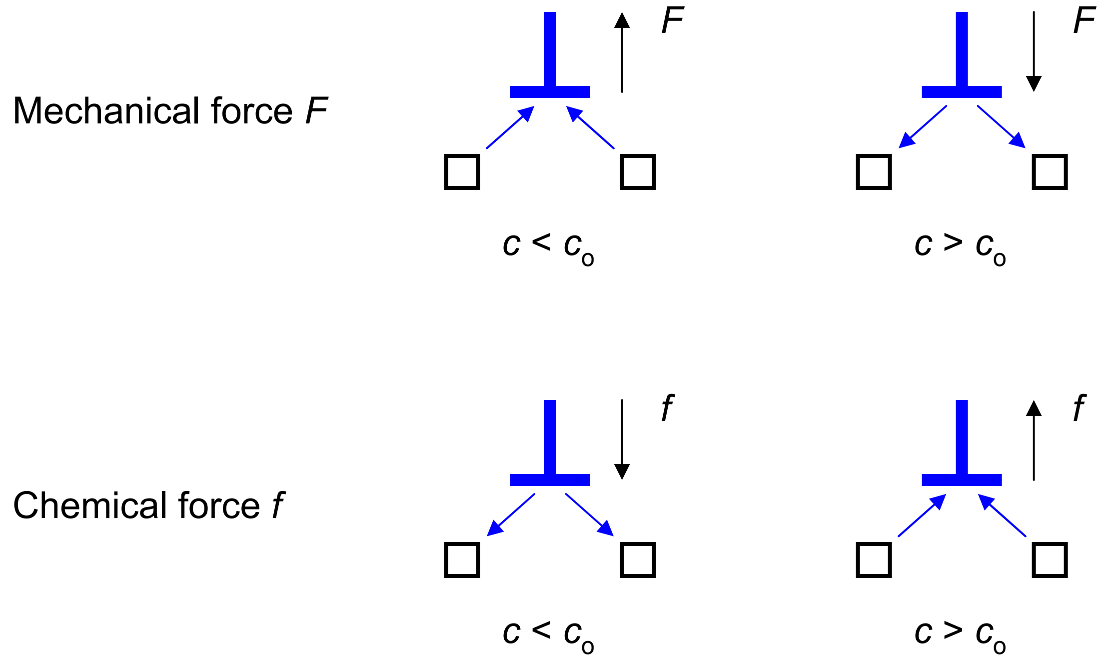
Chemical Force

B*

Climb Force

Figure 4.15 Mechanical and chemical forces for climb of an edge dislocation. Vacancies (shown as squares) have a local concentration *c* in comparison with the equilibrium concentration c_o in a dislocation-free crystal.

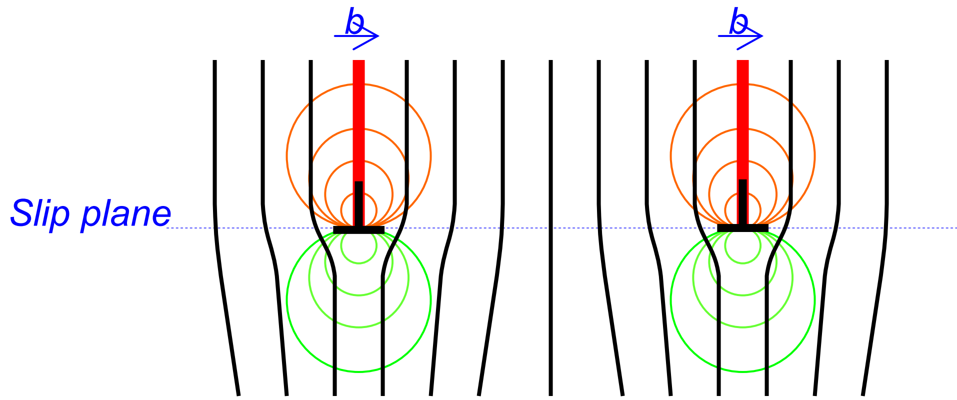
From D. Hull and D.J. Bacon, *Introduction to Dislocations, 4th Ed.*, (Butterworth-Heinemann, Oxford, 2001).



- For negative climb which involves vacancy emission (*i.e.*, $F < 0$), the sign of the chemical potential changes so that $c > c_o$. This causes f to build up to balance F in equilibrium.

- In the presence of a supersaturation of vacancies (c/c_o), the dislocation will climb up under the chemical force f until compensated by the mechanical force F (external stresses or line tension).

Implications of forces between dislocations (1)



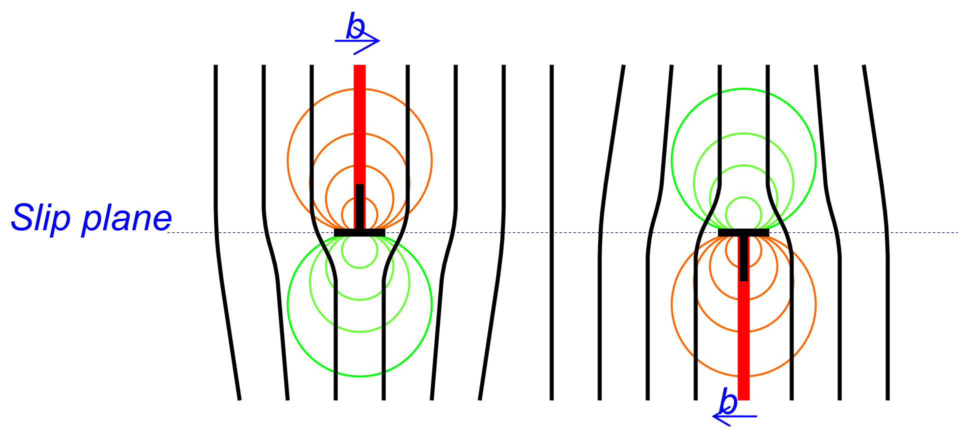
- Two like edge dislocations (i.e., both have parallel Burgers vectors) lying on the same slip plane will repel each other.

- We can approximate this from the equations developed for elastic strain energy.

$$E_{\text{elastic}} = \alpha G b^2 + \alpha G b^2 = \alpha G (2b)^2$$

Note the increased elastic strain energy

Implications of forces between dislocations (2)

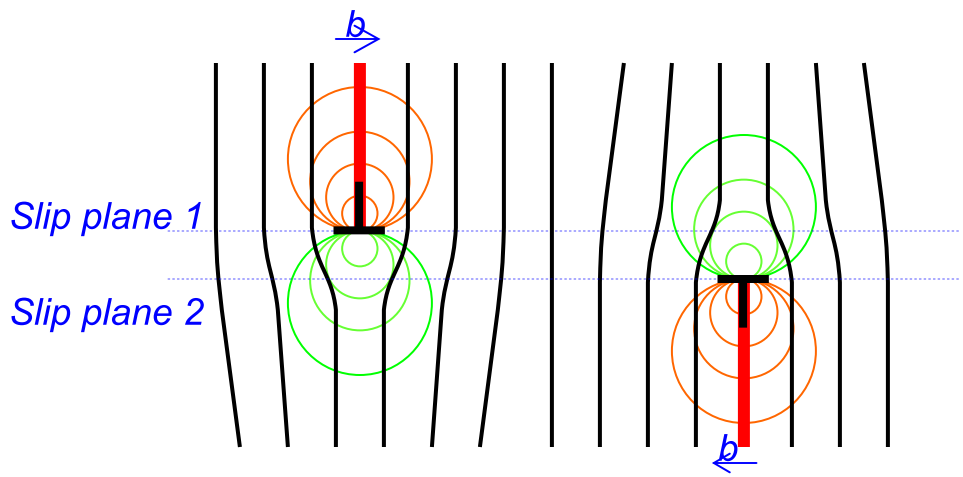


- Two unlike edge dislocations (i.e., both have opposite Burgers vectors) lying on the same slip plane will attract each other and annihilate out.

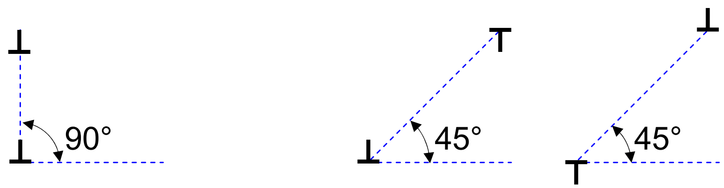
$$E_{\text{elastic}} = \alpha G b^2 - \alpha G b^2 = 0$$

Note the lack of elastic strain energy

Implications of forces between dislocations (3)



- Two unlike edge dislocations (i.e., both have opposite Burgers vectors) lying parallel slip planes separated by a few atomic spacings will attract each other and annihilate out leaving vacancies.



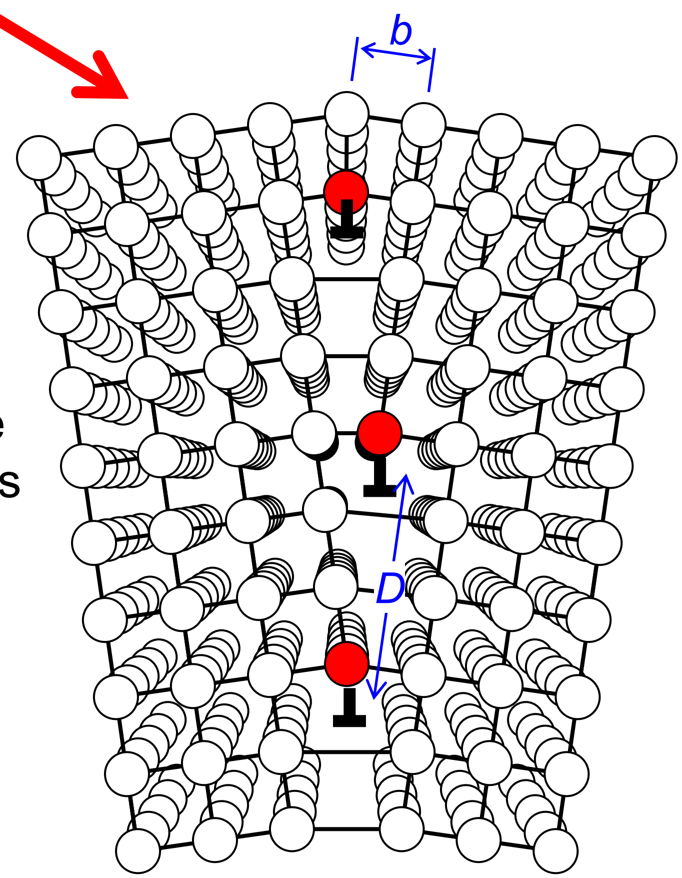
Same sign

Opposite sign

Stable positions for two edge dislocations

This results in unique configurations of dislocations.

Low-angle boundaries



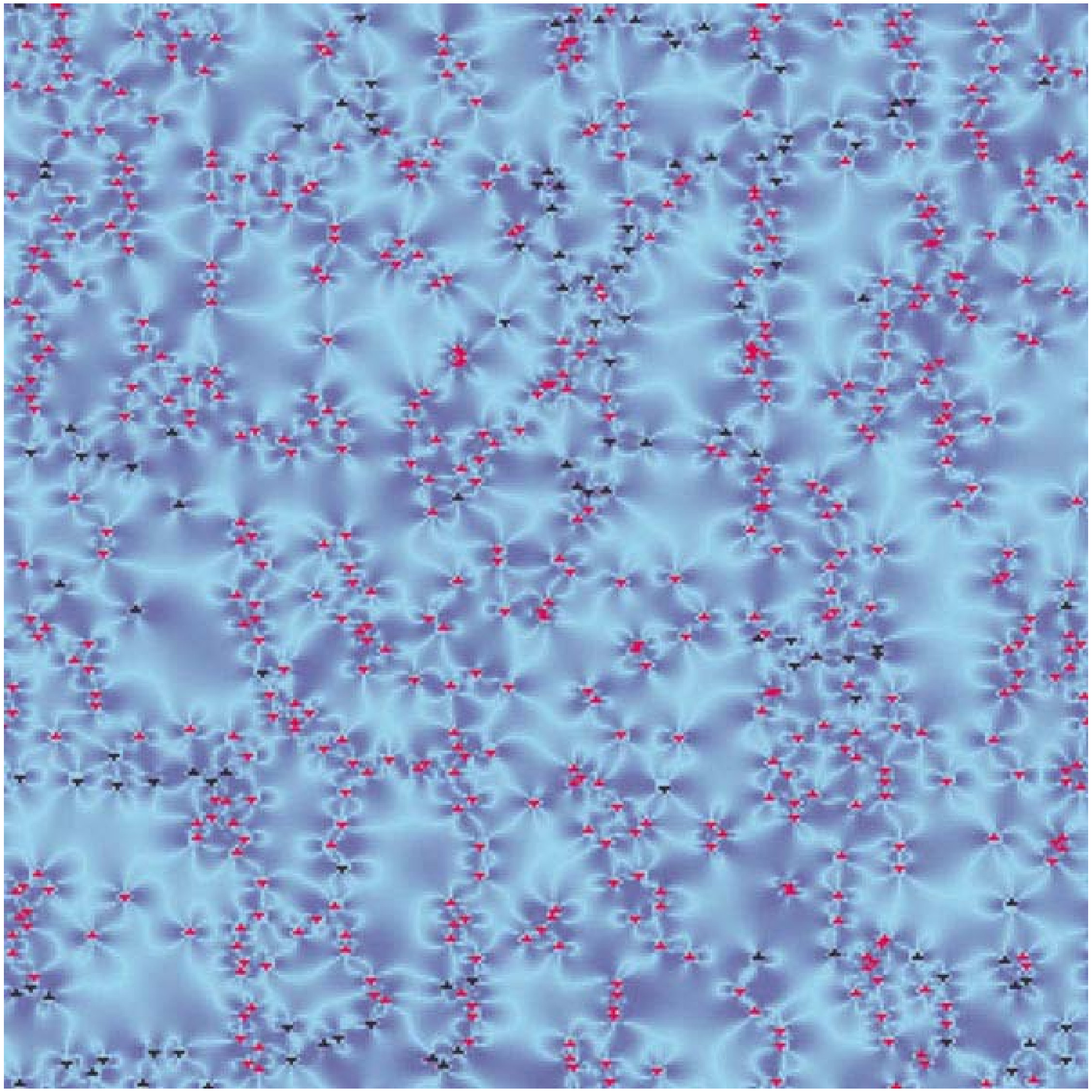


Figure 2
Numerical simulation of the total stress field and arrangement of dislocations in a solid.

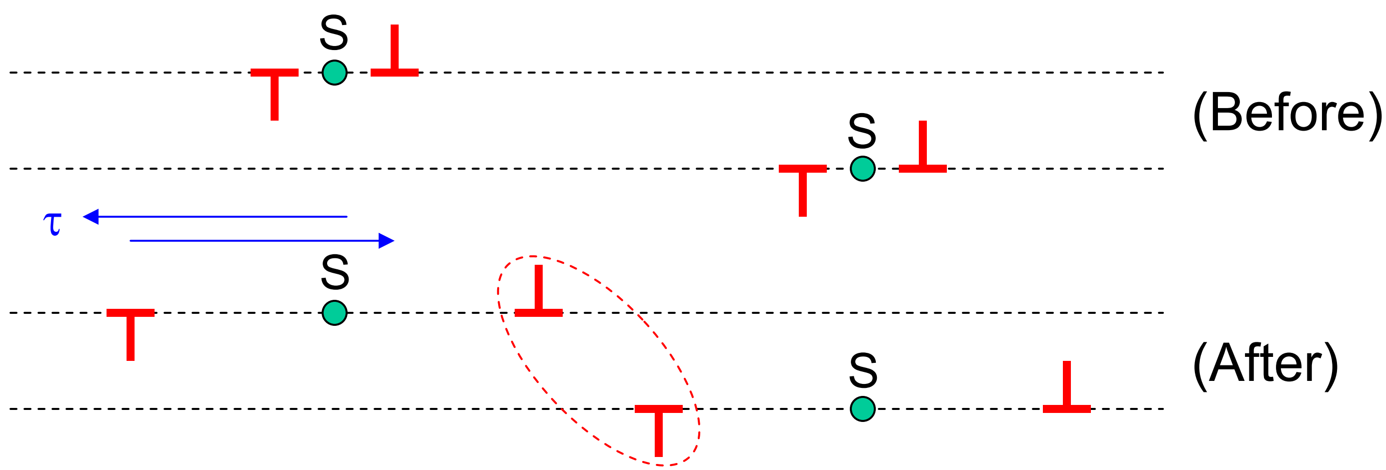
[M.-C. Miguel, A. Vespignani, S. Zapperi, J. Weiss and J.-R. Grasso, *Nature* v. 410, pp. 667-671(5 April 2001).]

The elastic stress fields around dislocations will interact either to repel or annihilate each other and to minimize elastic strain energy and obtain an equilibrium configuration.

Implications of forces between dislocations (7)

- Consider two dislocation sources (S) operating on parallel slip planes

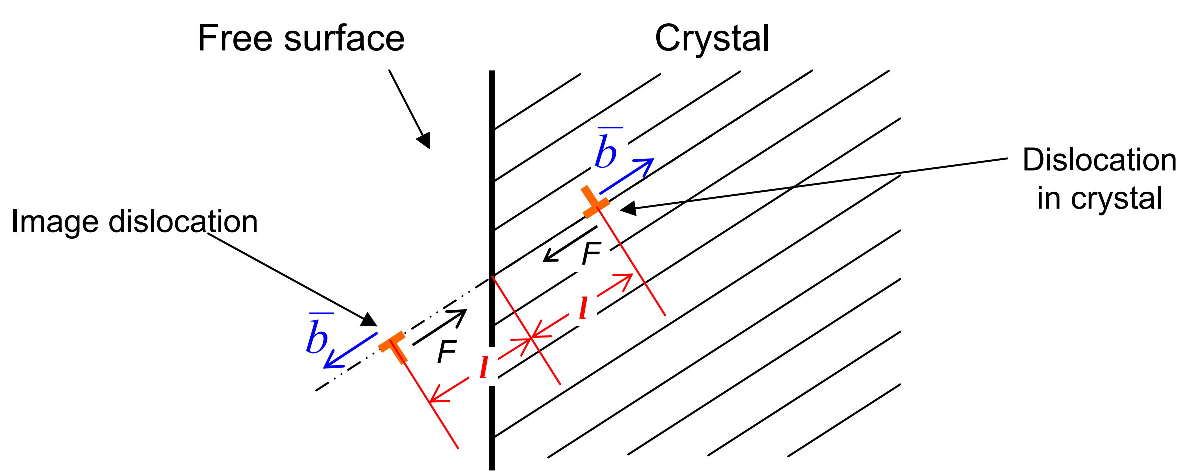
Dislocation dipoles and work hardening



- After application of a stress, the two circled segments will interact positively leading to a stable (45°) dislocation configuration for the two unlike segments. Once in this orientation, the two segments can no longer move past each other. The dislocations become locked. Slip is inhibited.
- This leads to hardening due to a reduction in dislocation mobility and a reduction in mobile dislocation density.

Forces between Dislocations and Free Surfaces

- Image forces
  - Free surfaces offer no stress in opposition to the displacements caused by an approaching dislocation.
  - Strain energy of the crystal decreases as a dislocation approaches a free surface. This pulls the dislocation towards the free surface (i.e., it “pulls the dislocation out of the crystal.



  - Another image and appropriate mathematics are detailed on the next 2 pages.

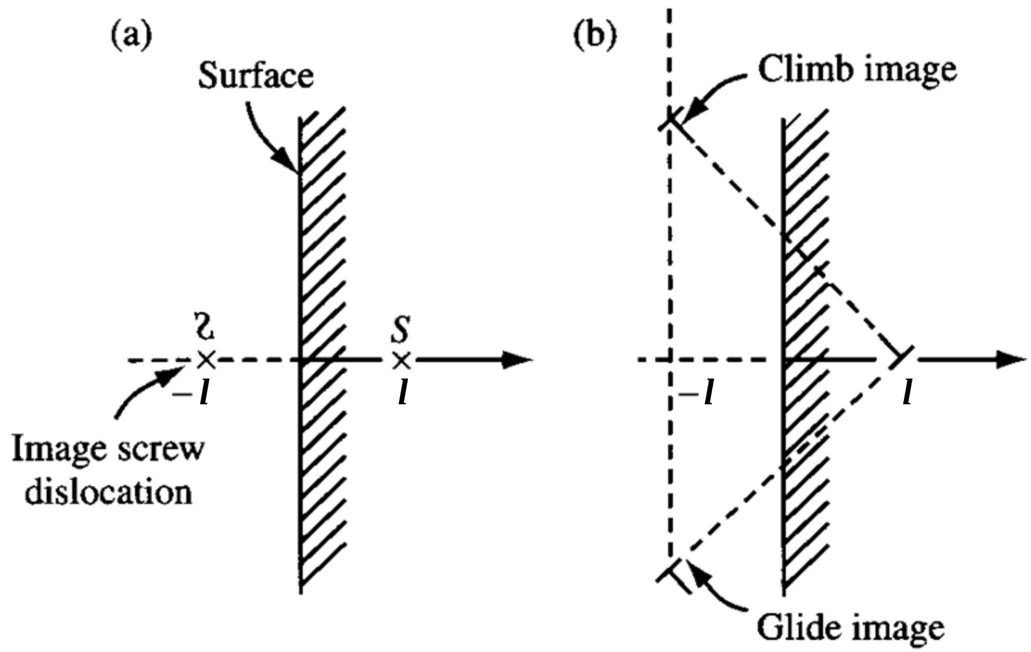


FIG. 2.5. (a) A negative image screw dislocation positioned at a distance $-a$ outside a surface both cancels the stresses of a positive screw dislocation a distance a under the surface and represents properly the force that a free surface exerts on the screw dislocation in the solid; (b) glide and climb images of an opposite edge dislocation, positioned as shown outside the solid, represent properly the forces exerted by the surface on the edge dislocation inside the solid but do not render the surface stress-free.

[Adapted from Argon, p. 37 (with modification)]

Screw Dislocation

$$\sigma_{zx} = \tau_{zx} = -\frac{Gb}{2\pi}\frac{y}{\left[(x-l)^2 + y^2\right]} + \frac{Gb}{2\pi}\frac{y}{\left[(x+l)^2 + y^2\right]}$$

and

$$\sigma_{zy} = \tau_{zy} = \frac{Gb}{2\pi}\frac{(x-l)y}{\left[(x-l)^2 + y^2\right]} - \frac{Gb}{2\pi}\frac{y}{\left[(x+l)^2 + y^2\right]}$$

at $x = l$, $y = 0$, the force on the screw dislocation is:

$$F_x = \tau_{zx} b = -\frac{Gb^2}{4\pi l}$$

Edge Dislocation

$$\sigma_{yx} = \tau_{yx} = \frac{Gb(x-l)\left[(x-l)^2 - y^2\right]}{2\pi(1-\nu)\left[(x-l)^2 + y^2\right]^2} - \frac{Gb(x+l)\left[(x+l)^2 + y^2\right]}{2\pi(1-\nu)\left[(x+l)^2 + y^2\right]^2}$$

$$-\frac{2Gbl\left[(x-l)(x+l)^3 - 6x(x+l)y^2 + y^4\right]}{2\pi(1-\nu)\left[(x+l)^2 + y^2\right]^3}$$

at $x = l$, $y = 0$, the force on the edge dislocation is:

$$F_x = \tau_{yx} b = -\frac{Gb^2}{4\pi(1-\nu)l}$$