

# 재료의 기계적 거동 (Mechanical Behavior of Materials)

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**Dislocations: elastic properties**

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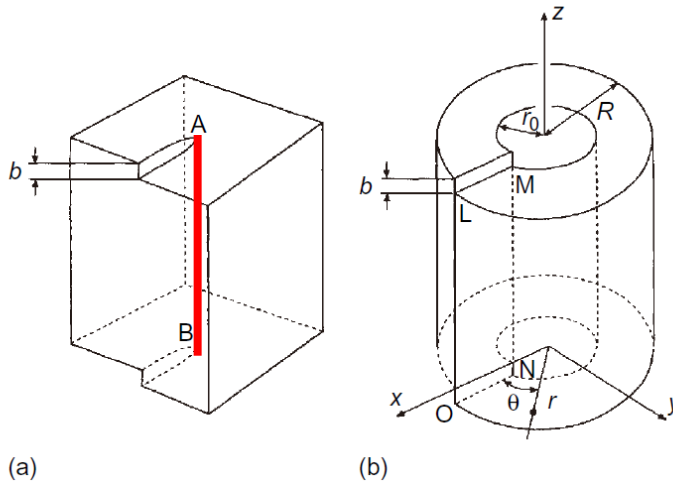
# Introduction

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- ◆ Dislocations are **line defects**. Thus, they distort the perfect crystal lattice.
- ◆ This lattice distortion **increases the free energy of the crystal lattice**. This is a direct result of **the elastic strain fields** that surround dislocations.
- ◆ **Interactions between the strain fields** (i.e., the distorted regions) around dislocations (and those of other defects) ultimately **determines the mechanical properties** of the lattice.

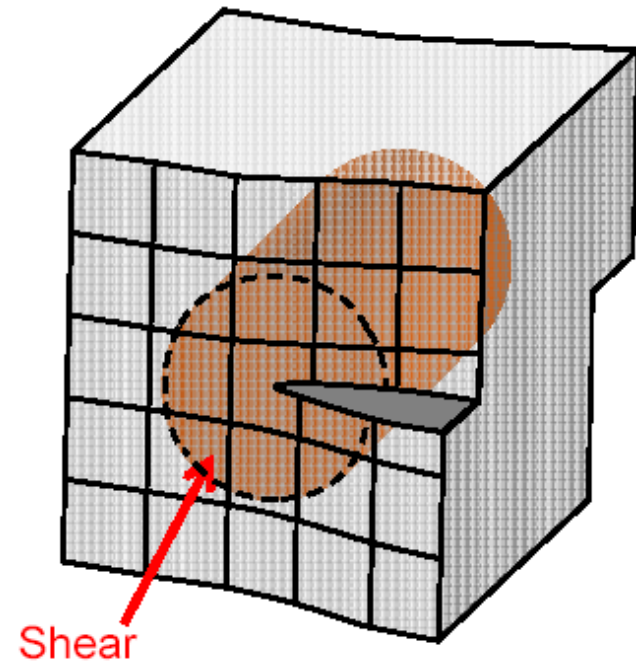


# Stress field of a straight screw dislocation



**FIGURE 4.5**

(a) Screw dislocation  $AB$  formed in a crystal. (b) Elastic distortion of a cylindrical tube simulating the distortion produced by the screw dislocation in (a).



Near the center of the dislocation 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  $r_0$ , we can model things using elasticity theory. Hooke's law applies here.  $r_0$  is called the *cutoff radius*. It typically has a value near  $b$ .

# Stress field of a straight screw dislocation

$$\begin{aligned}\varepsilon_{yz} &= \frac{1}{2}(u_{z,y} + u_{y,z}) \\ &= \frac{b \cos \theta}{4\pi r} \\ &= \frac{b x}{4\pi(x^2 + y^2)}\end{aligned}$$

$$\begin{aligned}\varepsilon_{xz} &= \frac{1}{2}(u_{z,x} + u_{x,z}) \\ &= -\frac{b \sin \theta}{4\pi r} \\ &= -\frac{b y}{4\pi(x^2 + y^2)}\end{aligned}$$

$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = \varepsilon_{xy} = 0$$

$$\begin{aligned}\sigma_{yz} &= \frac{Gb}{2\pi} \frac{x}{x^2 + y^2} \\ &= \frac{Gb \cos \theta}{2\pi r}\end{aligned}$$

$$\begin{aligned}\sigma_{xz} &= -\frac{Gb}{2\pi} \frac{y}{x^2 + y^2} \\ &= -\frac{Gb \sin \theta}{2\pi r}\end{aligned}$$

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

$$\varepsilon_{z\theta} = \frac{b}{4\pi r}$$



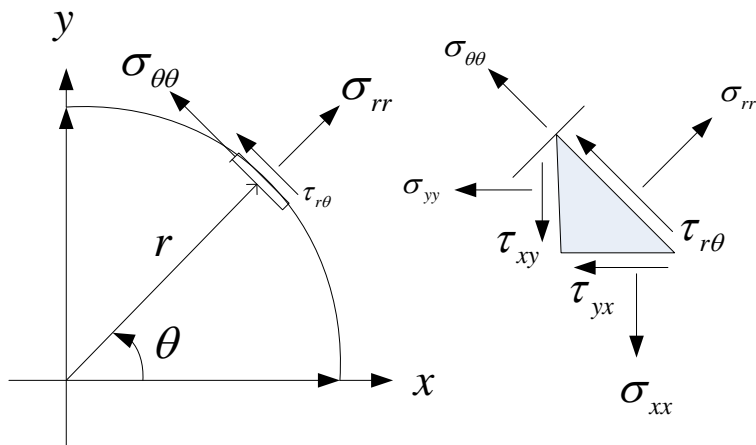
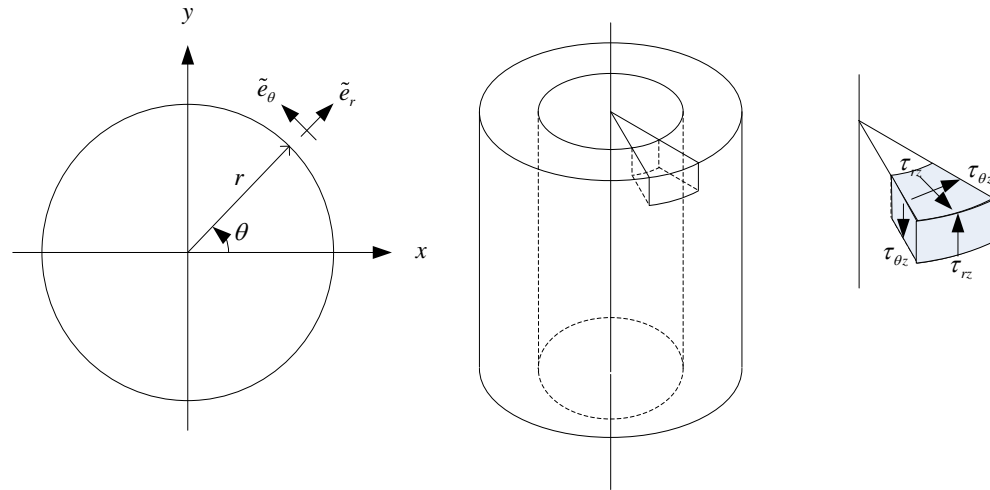
$$\sigma_{\theta z} = \frac{Gb}{2\pi r}$$



# Stress field of a straight screw dislocation

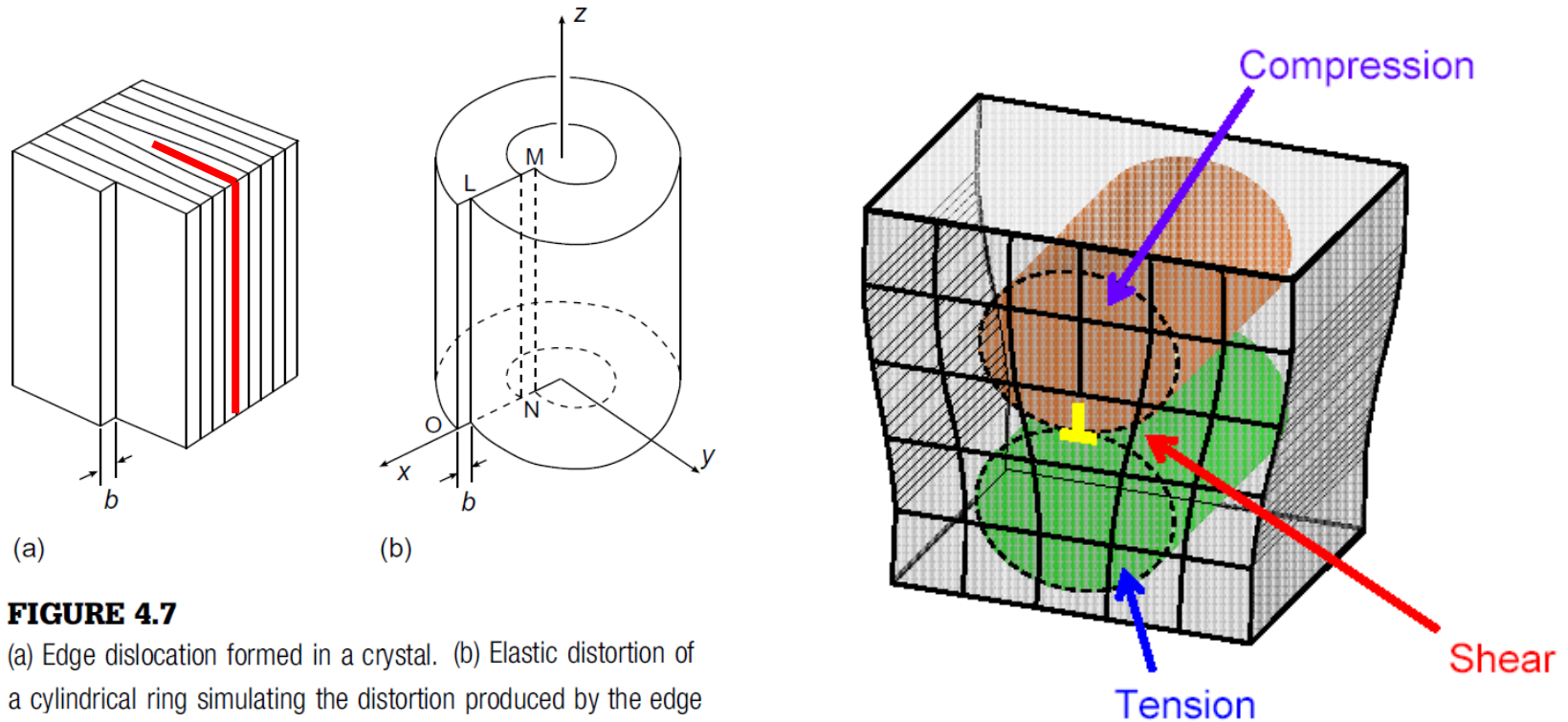
Cylindrical coordinate

$(r, \theta, z)$



$$\begin{aligned}\sigma_{rr} &= \sigma_{xx} \cos^2 \theta + \sigma_{yy} \sin^2 \theta + 2\tau_{xy} \sin \theta \cos \theta \\ \sigma_{\theta\theta} &= \sigma_{xx} \sin^2 \theta + \sigma_{yy} \cos^2 \theta - 2\tau_{xy} \sin \theta \cos \theta \\ \tau_{r\theta} &= (\sigma_{yy} - \sigma_{xx}) \sin \theta \cdot \cos \theta + \tau_{xy} (\cos^2 \theta - \sin^2 \theta) \\ \sigma_{zz} &= \sigma_{zz} \\ \sigma_{rz} &= \sigma_{xz} \cos \theta + \sigma_{yz} \sin \theta \\ \sigma_{\theta z} &= -\sigma_{xz} \sin \theta + \sigma_{yz} \cos \theta\end{aligned}$$

# Stress field of a straight edge dislocation



**FIGURE 4.7**

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

The pure edge dislocation has a **plane strain condition** since the displacement along the dislocation line,  $u_z$ , is absent. The stress field around a straight edge dislocation is obtained from the equilibrium condition.

# Stress field of a straight edge dislocation

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

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

$$\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$$

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

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

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

$$\sigma_{rr} = \sigma_{\theta\theta} = -\frac{Gb}{2\pi(1-\nu)} \frac{\sin\theta}{r}$$

$$\sigma_{zz} = \nu(\sigma_{rr} + \sigma_{\theta\theta}) = -\frac{Gb\nu}{\pi(1-\nu)} \frac{\sin\theta}{r}$$

$$\sigma_{r\theta} = \frac{Gb}{2\pi(1-\nu)} \frac{\cos\theta}{r}$$

$$\sigma_{zr} = \sigma_{\theta z} = 0$$

# Stress field of a straight edge dislocation

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

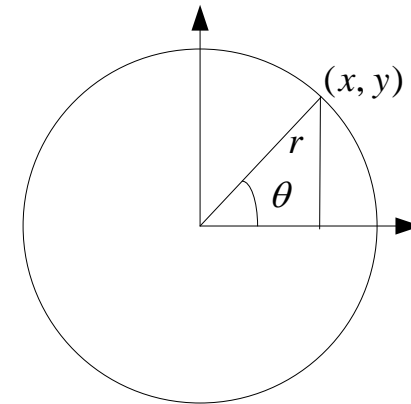
$$\sigma_{yy} = \frac{Gb}{2\pi(1-\nu)} \frac{y(x^2 - y^2)}{(x^2 + y^2)^2}$$

$$\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$$

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

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

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



$$\sigma_{xx} = -\frac{Gb}{2\pi r(1-\nu)} \sin \theta \cdot (2 + \cos 2\theta)$$

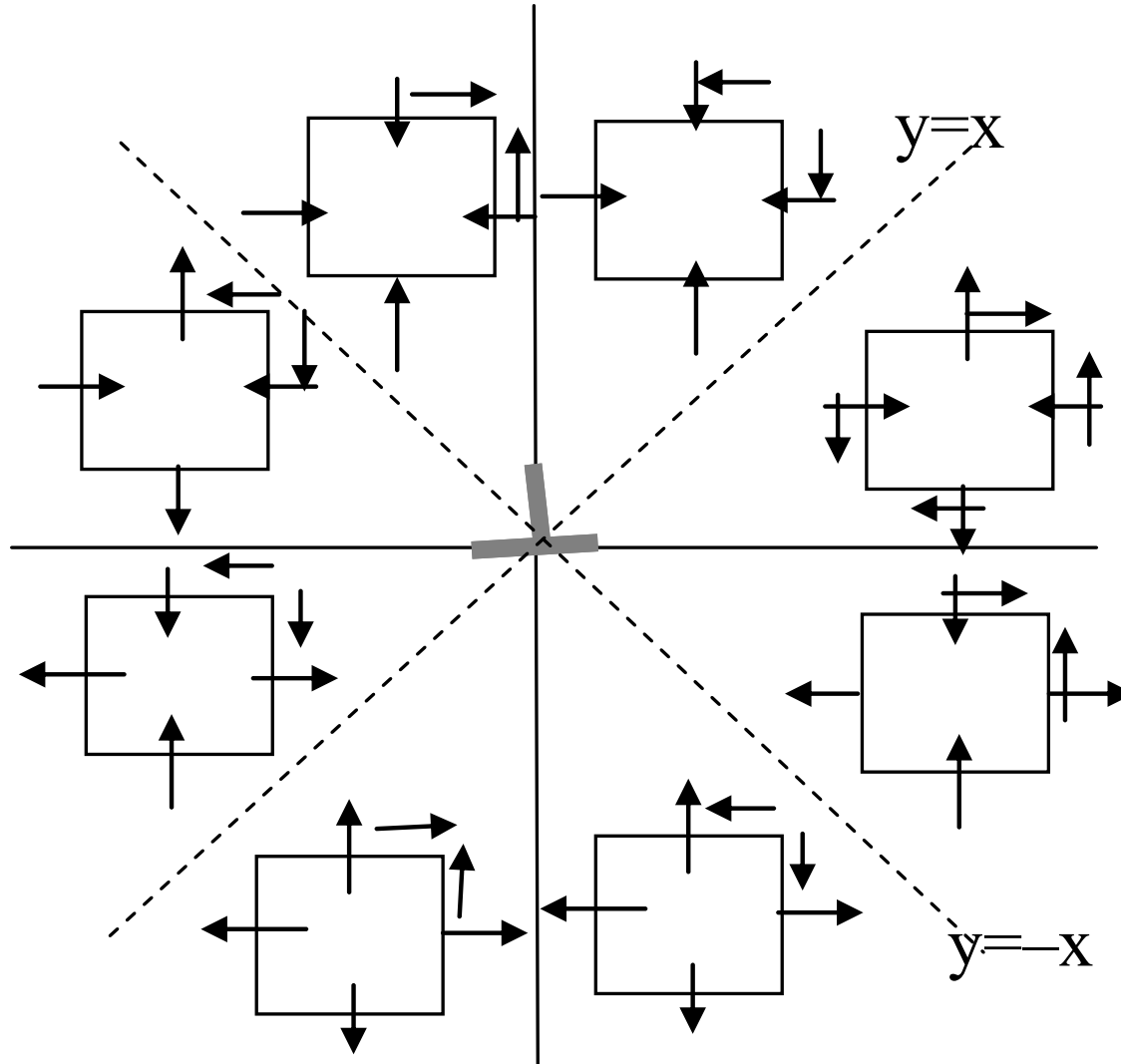
$$\sigma_{yy} = \frac{Gb}{2\pi r(1-\nu)} \sin \theta \cdot \cos 2\theta$$

$$\tau_{xy} = \tau_{yx} = \frac{Gb}{2\pi(1-\nu)r} \cos \theta \cdot \cos 2\theta$$

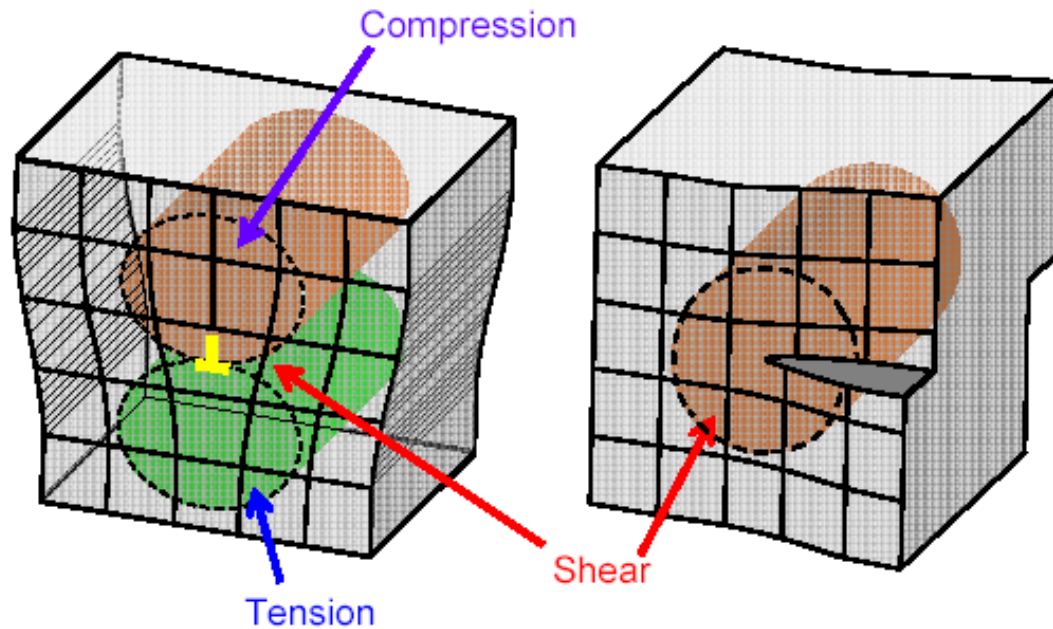
$$\sigma_{zz} = -\frac{Gb\nu}{\pi(1-\nu)r} \sin \theta$$



# Stress field of a straight edge dislocation



# Summary for straight dislocation



$$\sigma = \begin{pmatrix} E & E & S \\ E & E & S \\ S & S & E \end{pmatrix} \text{ in rectangular coordinate}$$

$$\sigma = \begin{pmatrix} E & E & 0 \\ E & E & S \\ 0 & S & E \end{pmatrix} \text{ in polar coordinate}$$

# Strain energy of a dislocation

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

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

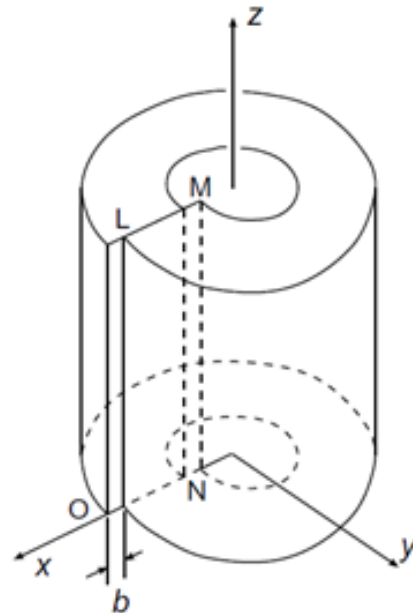
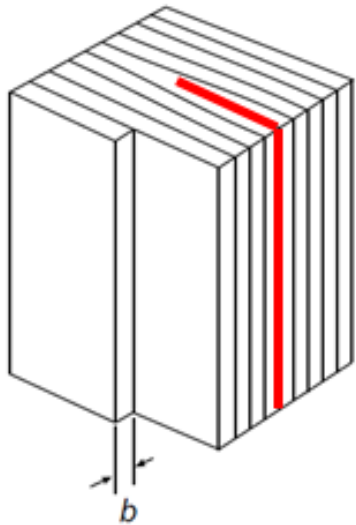
- The core contribution is difficult to calculate. It is estimated to have a value of  $\approx 0.5$  eV/plane threaded by a dislocation.

Elastic strain energy per unit length in screw dislocation

$$\begin{aligned} \frac{E_{\text{elast}}(\text{screw})}{l} &= \int_{r_0}^R 2G \frac{b^2}{(4\pi r)^2} 2\pi r dr \\ &= \frac{Gb^2}{4\pi} \int_{r_0}^R \frac{1}{r^2} dr = \boxed{\frac{Gb^2}{4\pi} \ln\left(\frac{R}{r_0}\right)} \end{aligned}$$

# Strain energy of a dislocation

Elastic strain energy per unit length in edge dislocation



$$dE_{el}(edge) = \frac{1}{2} \sigma_{xy} dA \cdot b$$

$$dA = dx \cdot l$$

$$\frac{E_{el}(edge)}{l} = \int_{r_0}^R \frac{1}{2} bD \frac{x(x^2 - y^2)}{(x^2 + y^2)^2} \Big|_{y=0} bdx$$

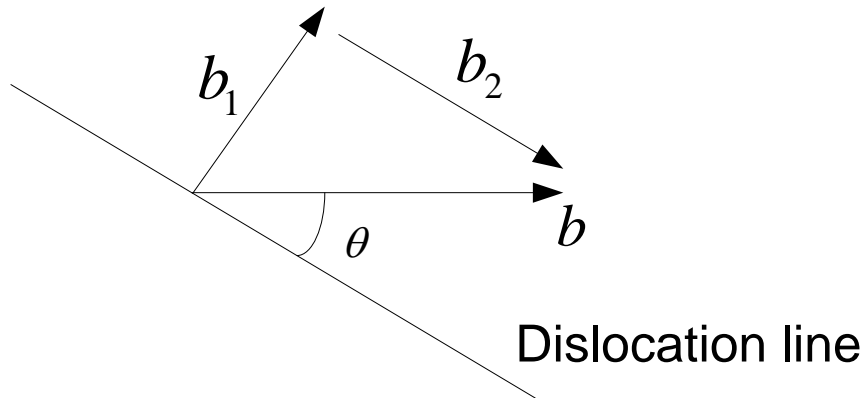
$$= \frac{bD}{2} \ln \left( \frac{R}{r_0} \right)$$

$$= \frac{Gb^2}{4\pi(1-\nu)} \ln \left( \frac{R}{r_0} \right)$$

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

# Strain energy of a dislocation

Elastic strain energy per unit length in mixed dislocation



$$b_1 = b \sin \theta \quad (\text{edge})$$

$$b_2 = b \cos \theta \quad (\text{screw})$$

$$\frac{E_{el}(\text{mixed})}{l} = \left( \frac{Gb^2 \cos^2 \theta}{4\pi} + \frac{Gb^2 \sin^2 \theta}{4\pi(1-\nu)} \right) \ln \left( \frac{R}{r_0} \right)$$

# Strain energy of a dislocation

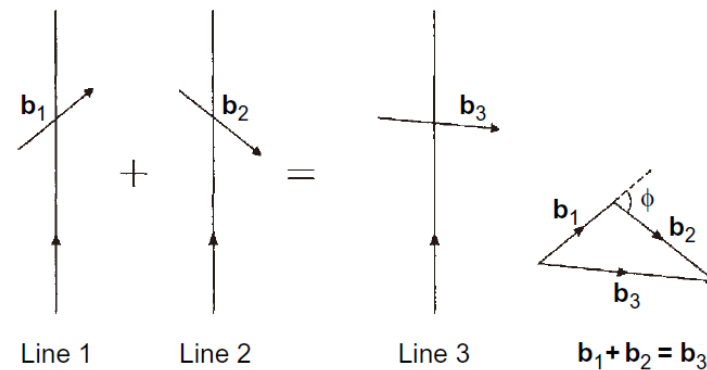
- One of the important consequences of this relationship is that it allows us to determine whether or not it is energetically feasible for two dislocations to react and combine to form another. This is known as Frank's Rule.

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

where  $\alpha \approx 0.5 - 1.0$

OR

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



**FIGURE 4.9**

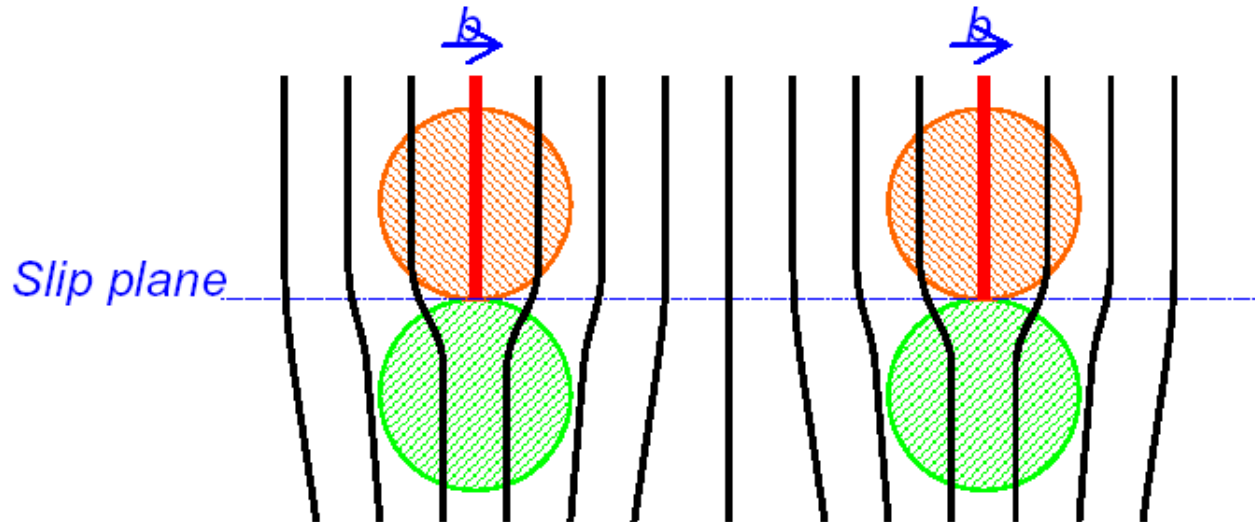
Reaction of two dislocations to form a third.

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

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

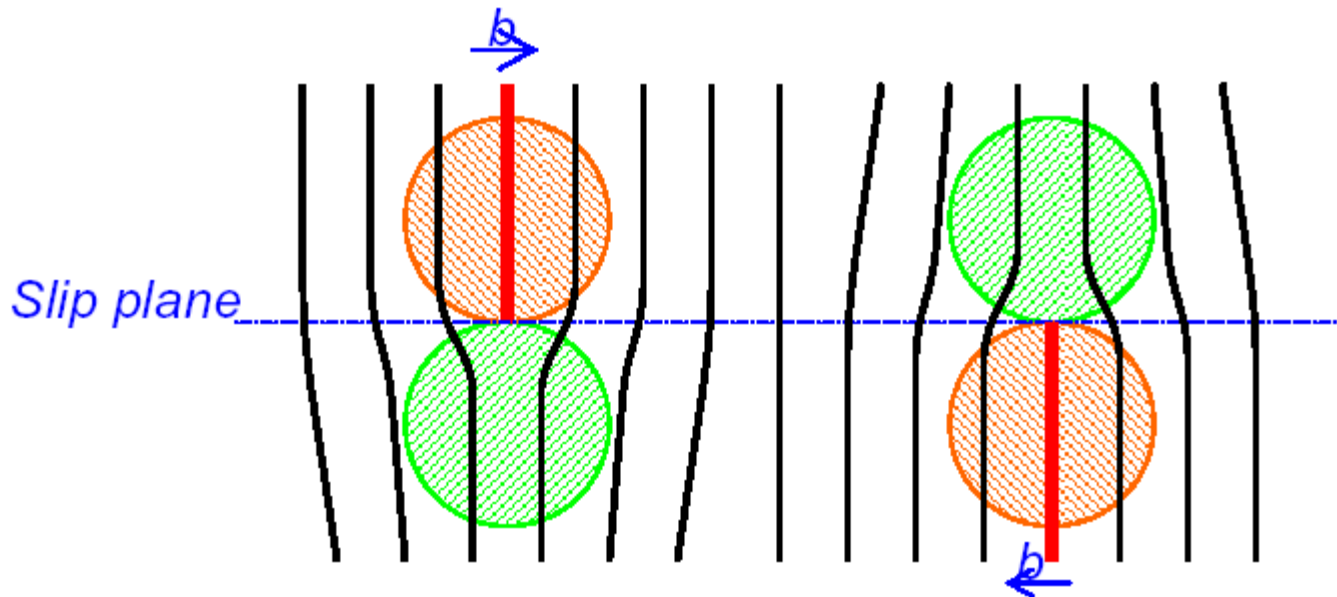
No net energy change if  $(b_1^2 + b_2^2) = b_3^2$

# Forces between dislocations



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

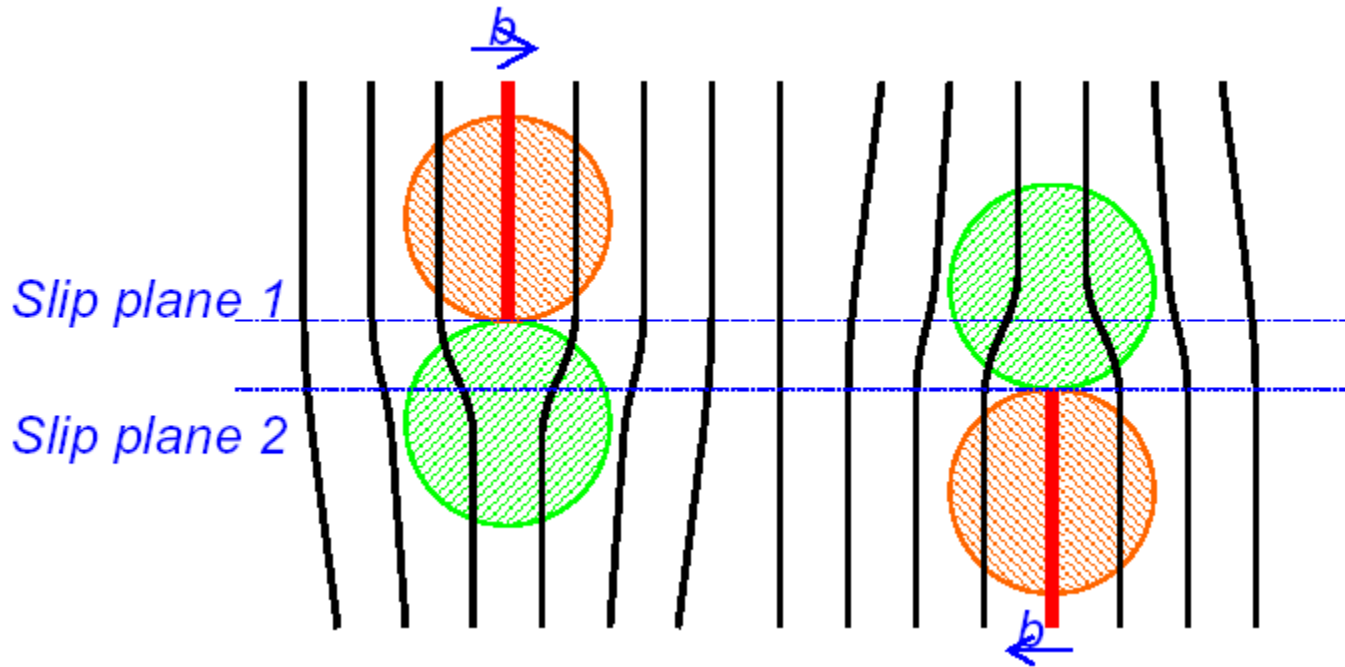
# Forces between dislocations



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

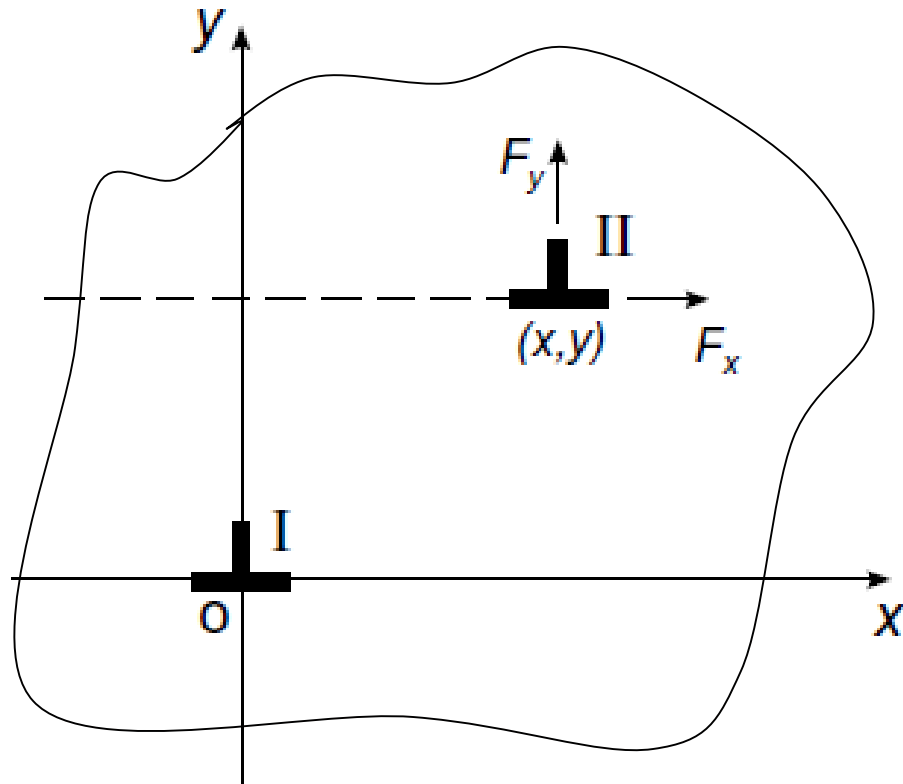


# Forces between dislocations



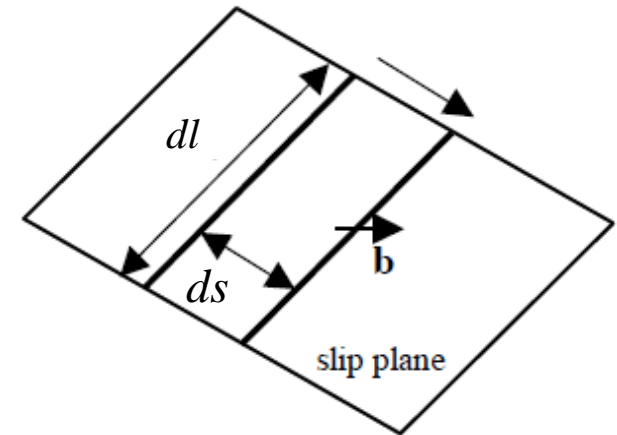
Two **unlike edge dislocations** (i.e., both have opposite Burgers vectors) lying **parallel slip planes separated by a few atomic spacings** will **attract** each other and **annihilate** out leaving **vacancies**.

# *What will happen when the dislocations adopt different configurations?*



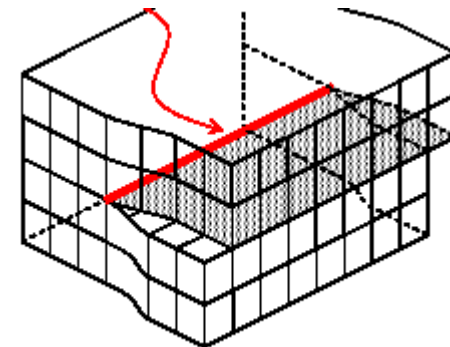
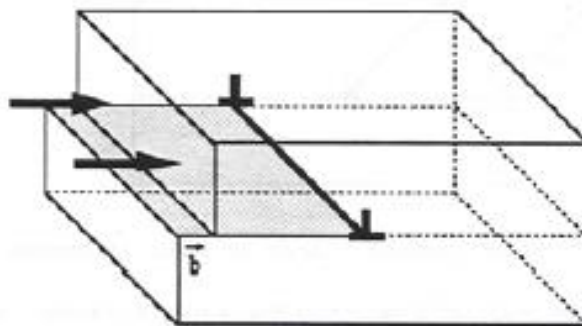
# Force Acting on a Dislocation

- Total area of slip plane :  $A$
- Average shear displacement :  $(dl ds/A)b$
- Shear force on slip plane :  $\tau A$
- Work done when the element of slip occurs :  
 $dW = \tau A (dl ds/A)b = \tau (dl ds)b$



- The glide force  $F$  on a unit length of dislocation  
 $F = dW/(dl ds) = dW/dA = \tau b$

*Glide force is always directed normal to the dislocation line.*



# *Peach-Koehler equation*

Applied stress :  $\boldsymbol{\sigma}$

Dislocation line vector (unit vector) :  $\mathbf{t}$



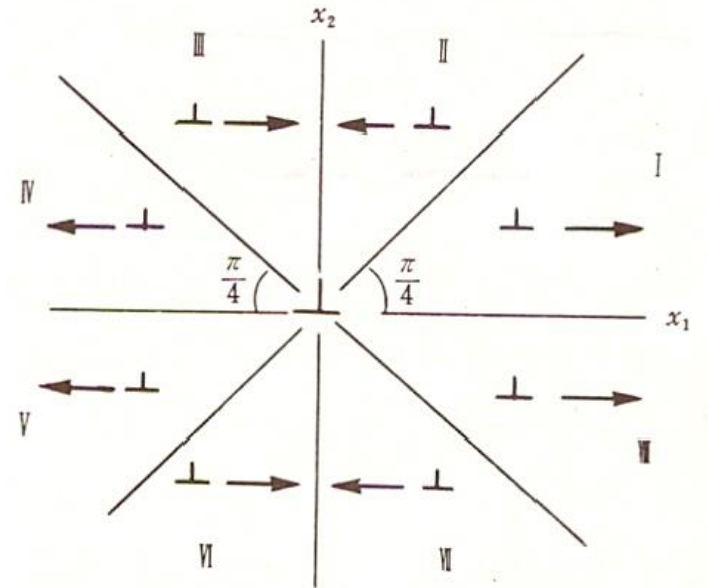
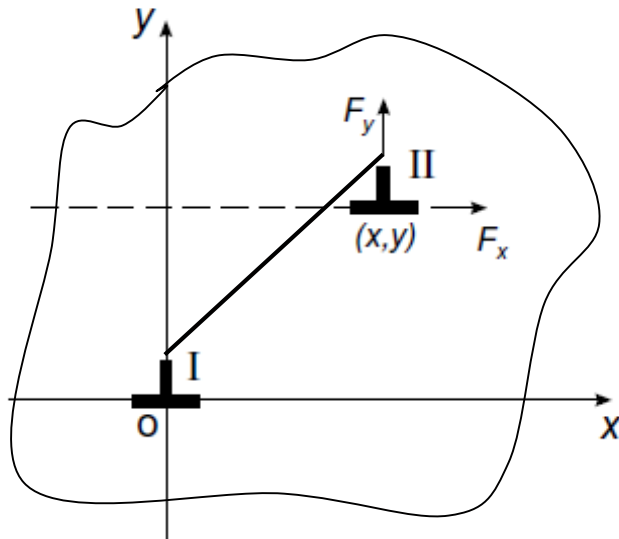
$$\mathbf{F} = (\boldsymbol{\sigma} \diamond \mathbf{b}) \times \mathbf{t}$$



$$\mathbf{F} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ G_1 & G_2 & G_3 \\ t_1 & t_2 & t_3 \end{vmatrix} \quad \begin{aligned} G_1 &= \sigma_{11}\mathbf{b}_1 + \sigma_{12}\mathbf{b}_2 + \sigma_{13}\mathbf{b}_3 \\ G_2 &= \sigma_{21}\mathbf{b}_1 + \sigma_{22}\mathbf{b}_2 + \sigma_{23}\mathbf{b}_3 \\ G_3 &= \sigma_{31}\mathbf{b}_1 + \sigma_{32}\mathbf{b}_2 + \sigma_{33}\mathbf{b}_3 \end{aligned}$$



# What will happen when the dislocations adopt different configurations?



$$F_x = \frac{Gbb'}{2\pi(1-\nu)r} \cos \theta \cos 2\theta$$

$$F_y = \frac{Gbb'}{2\pi(1-\nu)r} \sin \theta (2 + \cos 2\theta)$$

# What will happen when the dislocations adopt different configurations?

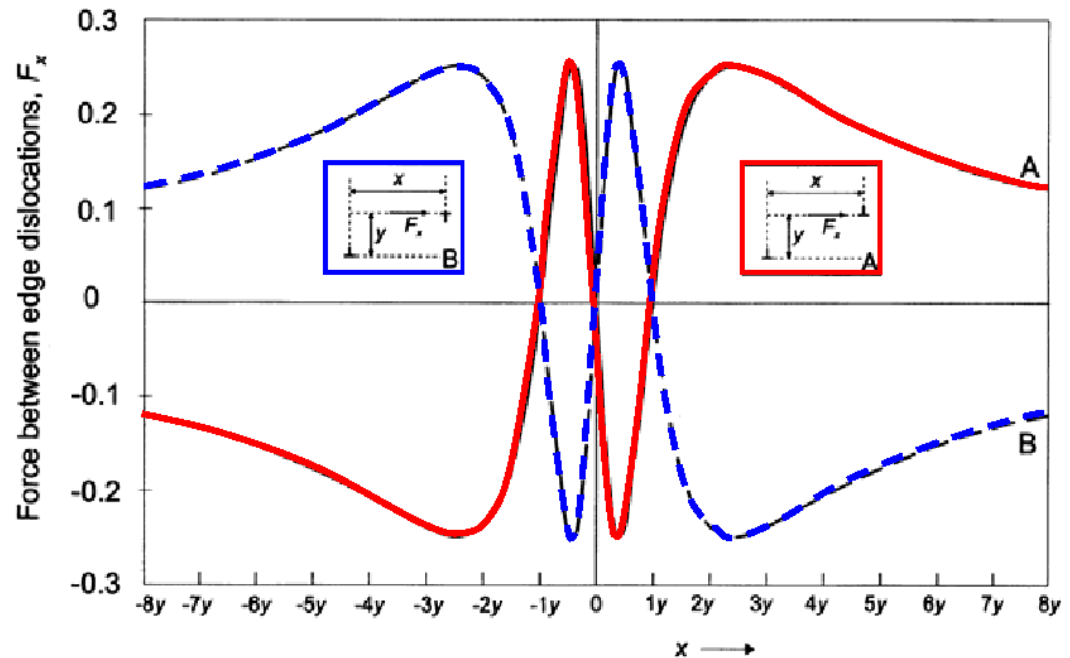
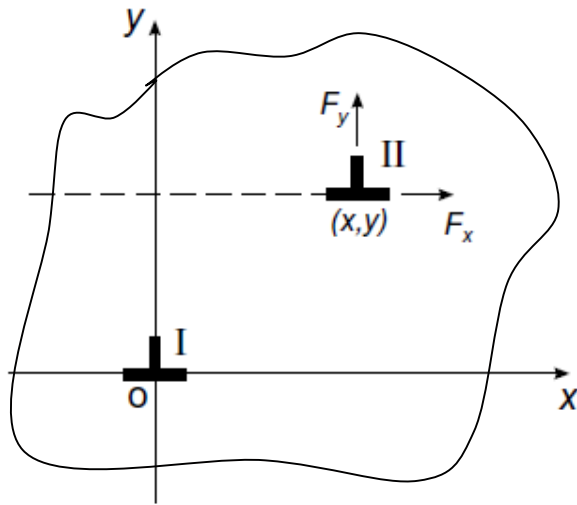
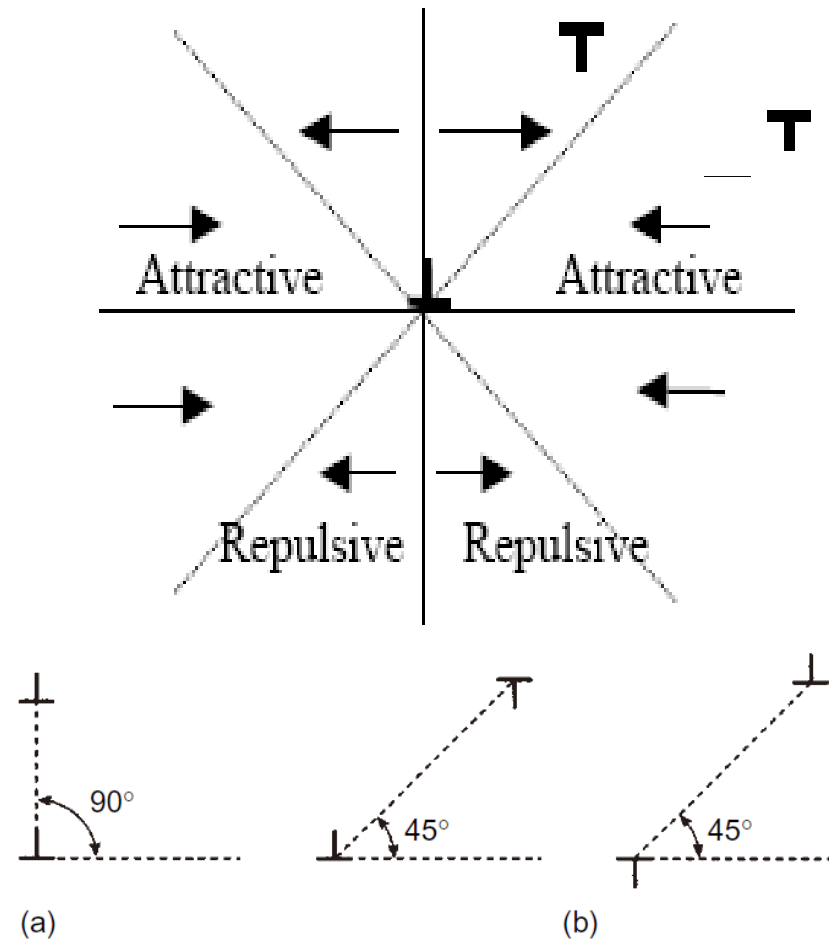


Figure 4.13 Glide force per unit length between parallel edge dislocations with parallel Burgers vectors from equation (4.36). Unit of force  $F_x$  is  $Gb^2/2\pi(1-\nu)y$ . The full curve *A* is for like dislocations and the broken curve *B* for unlike dislocations.

$$\mathbf{F} = b_1 \frac{Gb_2}{2\pi(1-\nu)} \frac{x(x^2 - y^2)}{(x^2 + y^2)^2} \mathbf{i} + b_1 \frac{Gb_2}{2\pi(1-\nu)} \frac{y(3x^2 + y^2)}{(x^2 + y^2)^2} \mathbf{j}$$

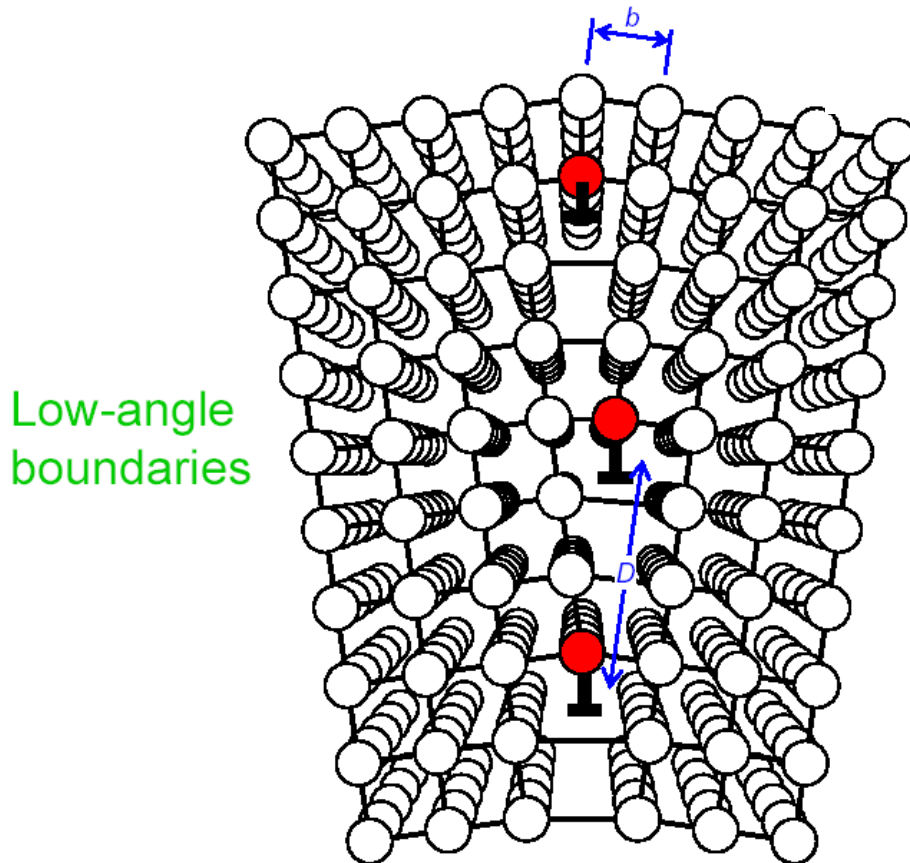
# What will happen when the dislocations adopt different configurations?



**FIGURE 4.15**

Stable positions for two edge dislocations of (a) the same sign and (b) opposite sign.

# What will happen when the dislocations adopt different configurations?



Screw dislocation :

$$\mathbf{F}_r = \frac{Gbb'}{2\pi r}$$