

Mechanical Behaviour of Materials

Chapter 05-1

Dislocation: Basics

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Theoretical strength of crystals

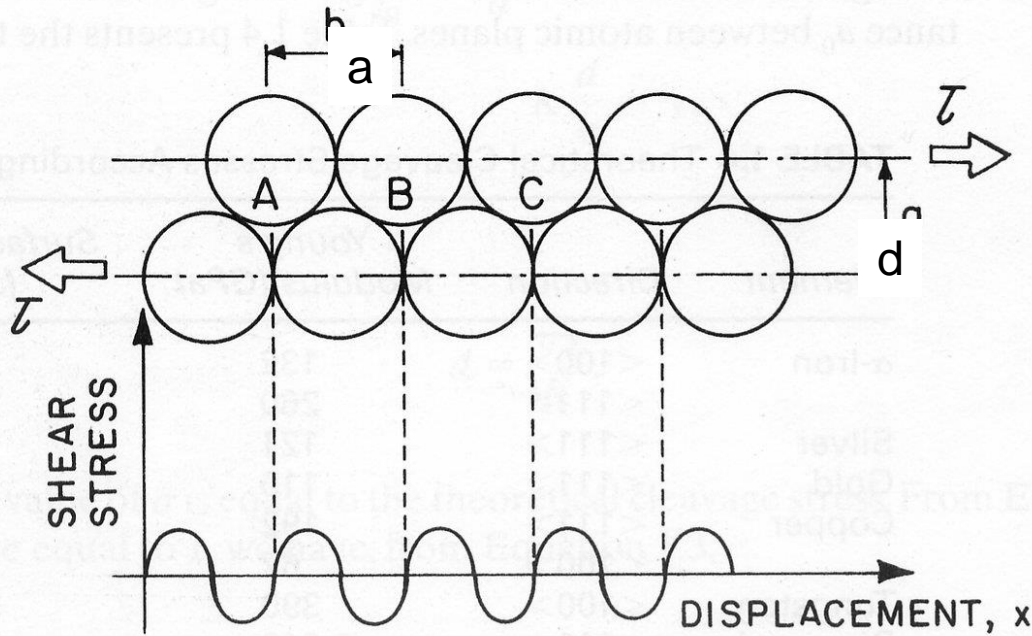


Figure 1.33 Stress required to shear a crystal.

According to Frenkel

$$\tau = \tau_{\max} \sin \frac{2\pi x}{a}$$

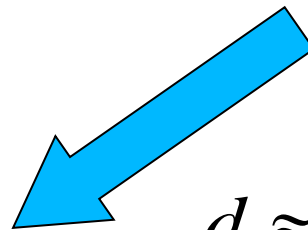
$$\tau \approx \tau_{\max} \frac{2\pi x}{a}$$

$$\tau = G \frac{x}{d}$$

$$\tau_{\max} = \frac{Ga}{2\pi d}$$

$$\tau_{\max} \approx \frac{G}{2\pi}$$

$$d \approx a$$



Is theoretical strength of crystals possible to achieve?

Why are the theoretical cleavage and shear strengths of materials possible to reach?

Table 9.1. Critical shear stress for slip in several materials

Metal	Purity %	Critical shear stress (MPa)	
		Experiment	Theory
copper	>99.9	1.0	414
silver	99.99	0.6	285
cadmium	99.996	0.58	207
iron	99.9	~7.0	740

Note: There is considerable scatter caused by experimental variables, particularly purity.

Is theoretical strength of crystals possible to achieve?

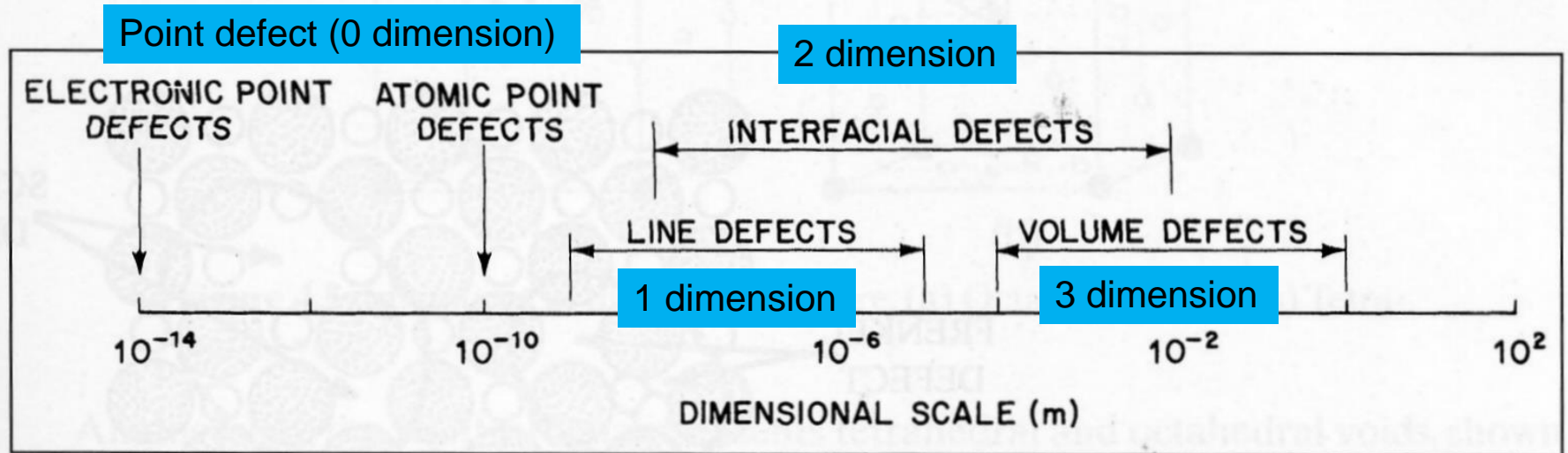
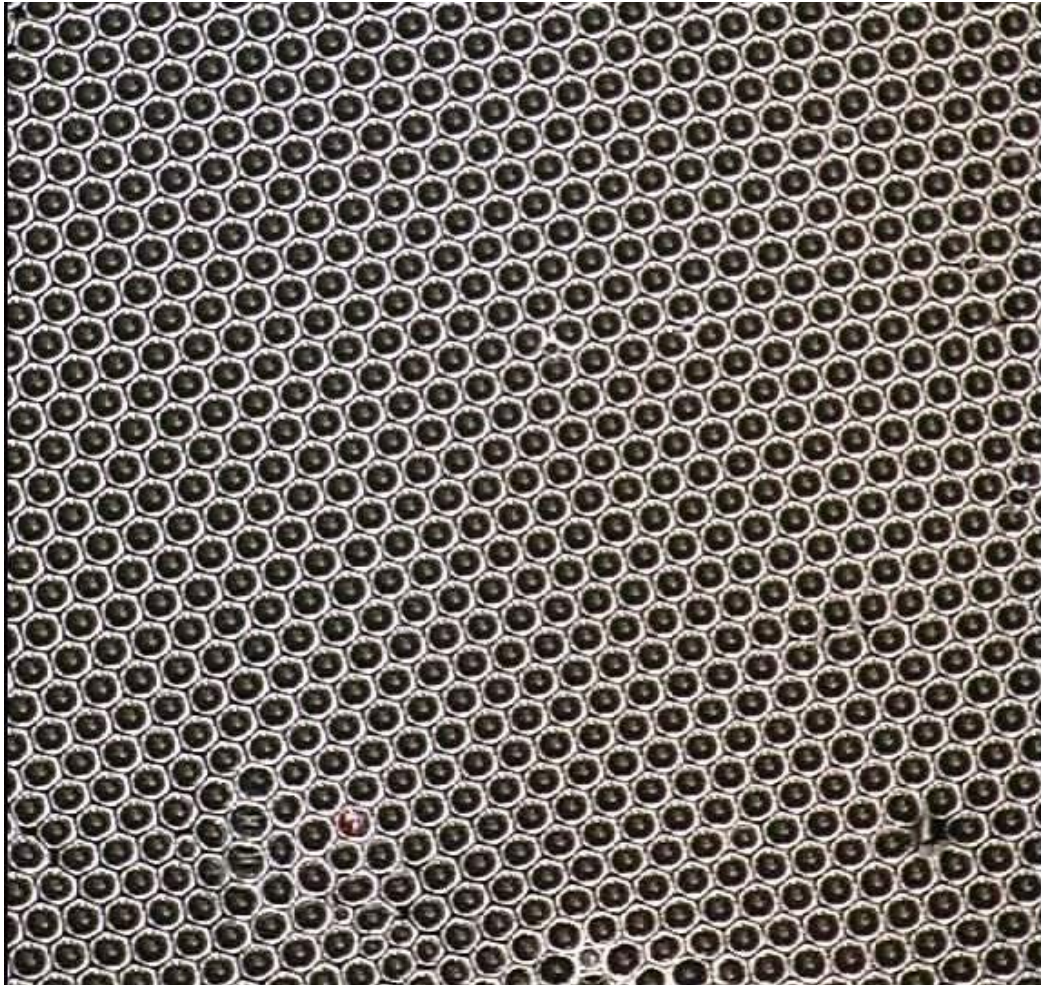


Figure 4.1 Dimensional ranges of different classes of defects.

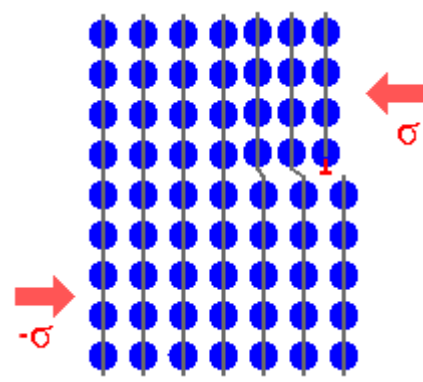
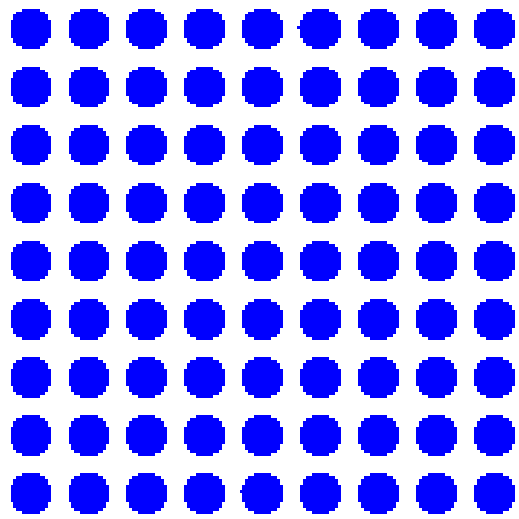
Why are the theoretical cleavage and shear strengths of materials possible to reach?

What kind of defects?

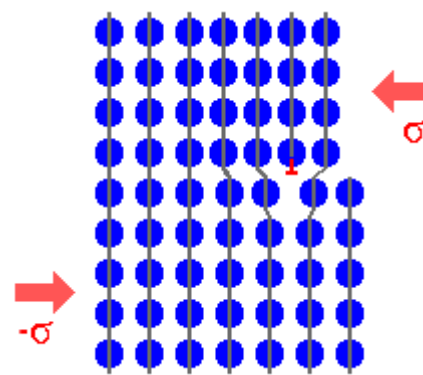


Is theoretical strength of crystals possible to achieve?

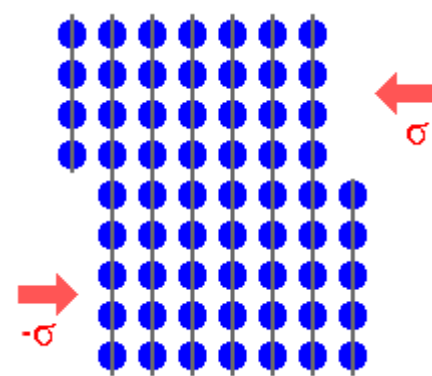
Dislocation movement and plastic deformation



Generation of an edge dislocation by a *shear* stress

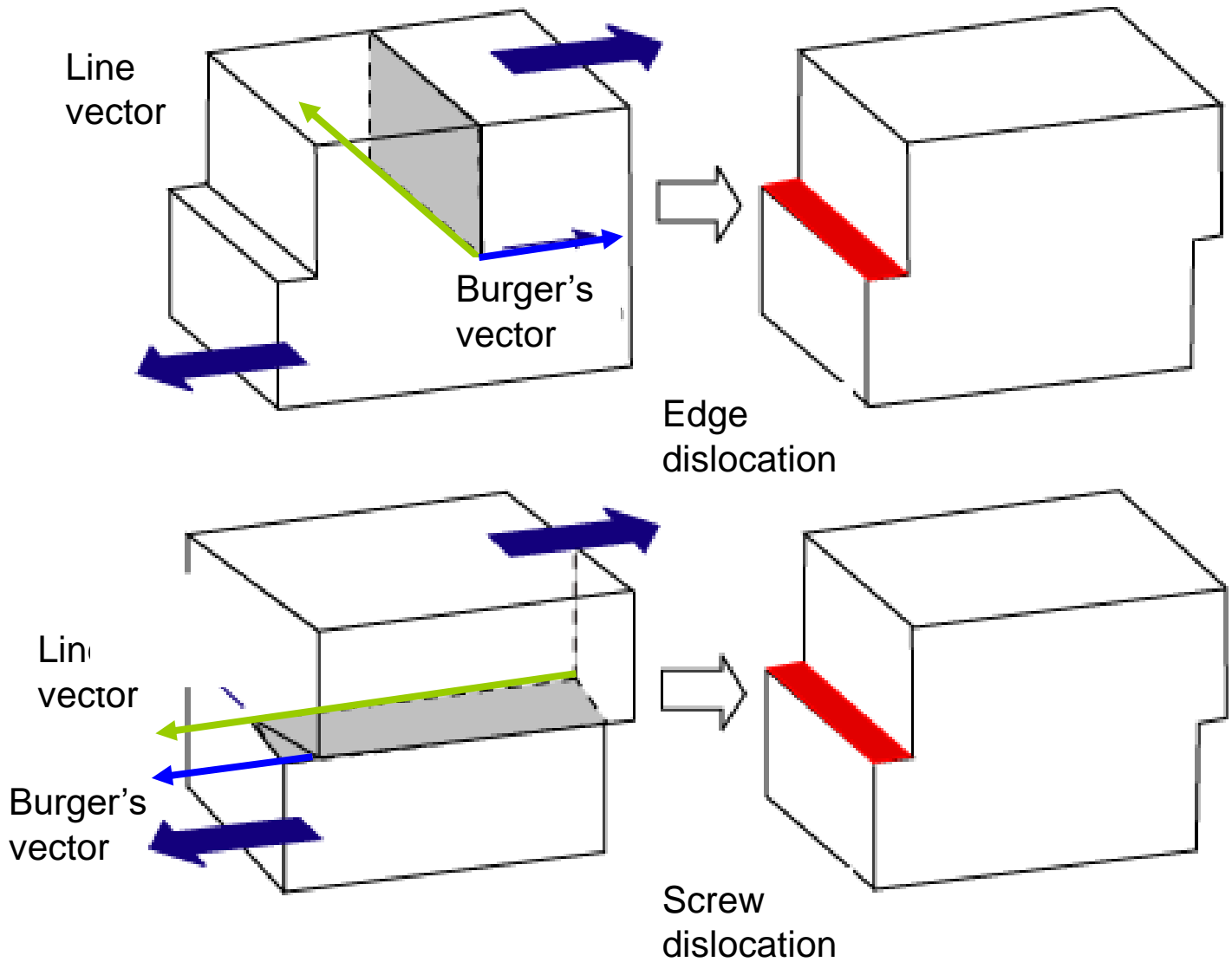


Movement of the dislocation through the crystal

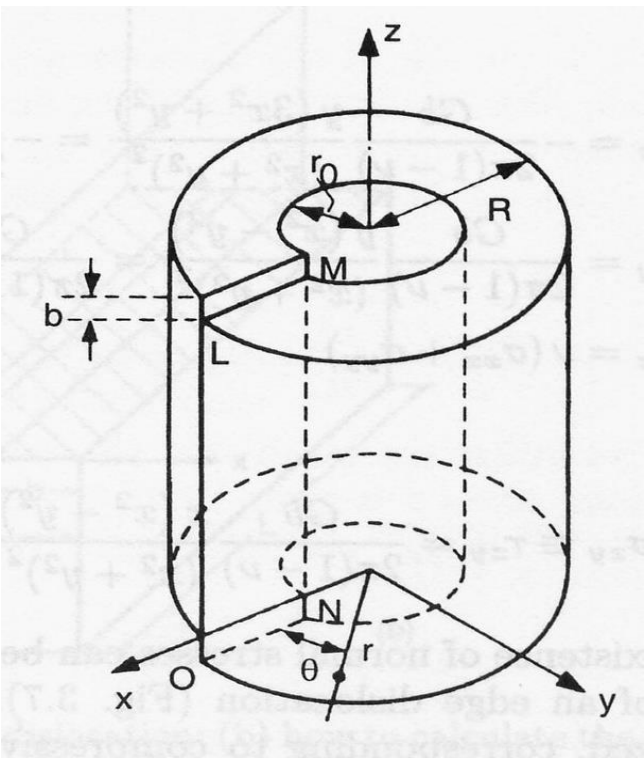
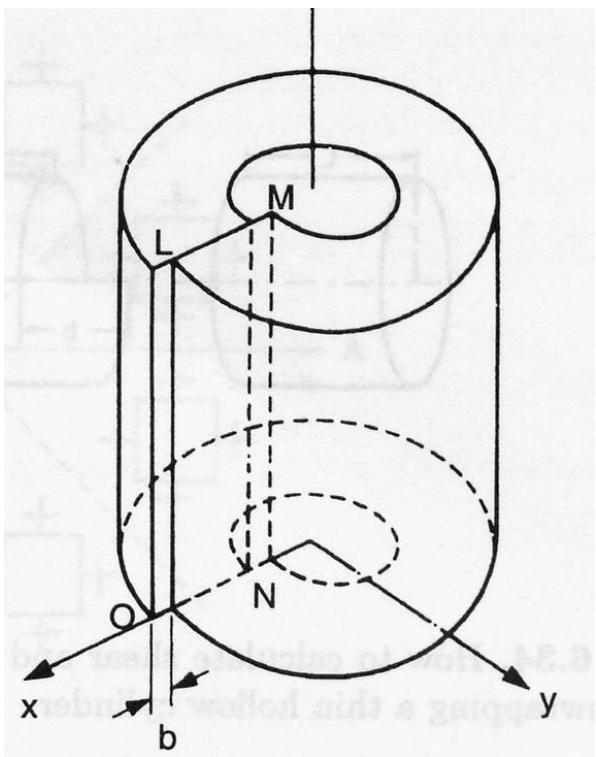


Shift of the upper half of the crystal after the dislocation emerged

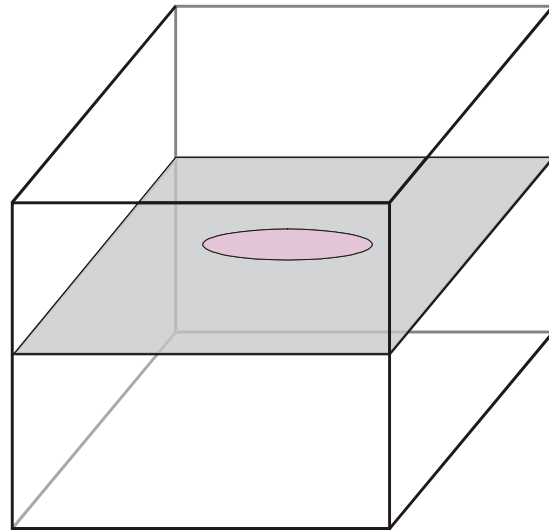
Definition of edge and screw dislocations



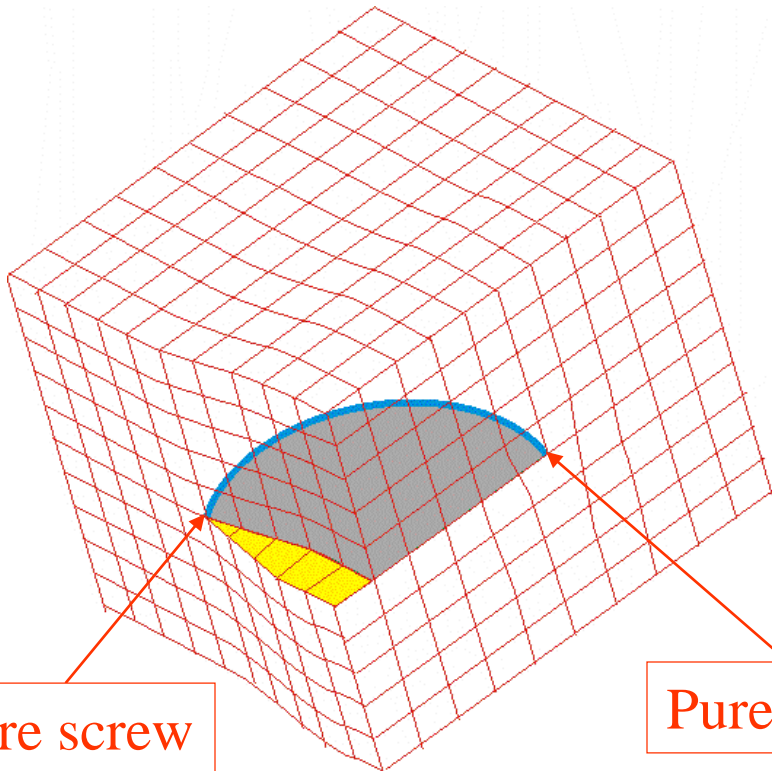
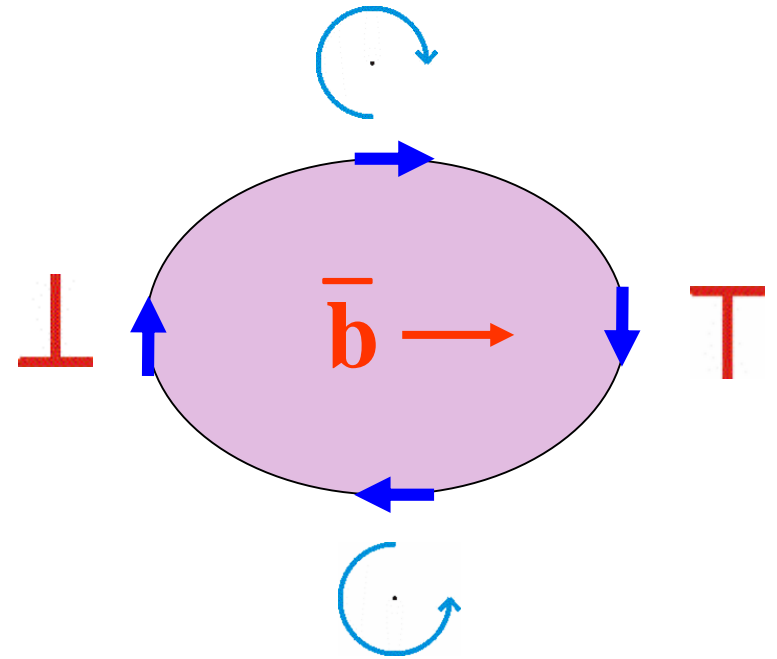
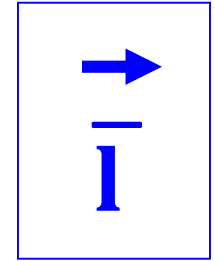
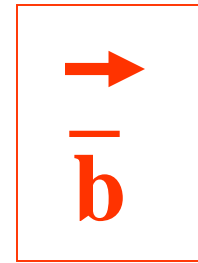
Definition of edge and screw dislocations



Mixing dislocations



Mixed dislocations



Pure screw

Pure Edge

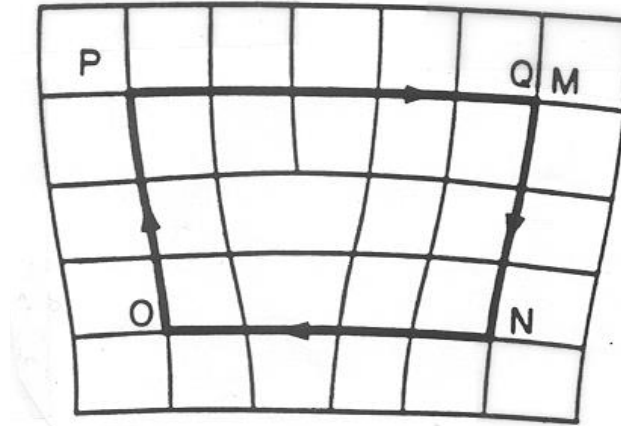
Summary

Dislocation Property	Type of dislocation	
	Edge	Screw
Relation between dislocation line (l) and b	\perp	\parallel
Slip direction	\parallel to b	\parallel to b
Direction of dislocation line movement relative to b	\parallel	\perp
Process by which dislocation may leave slip plane	climb	Cross-slip

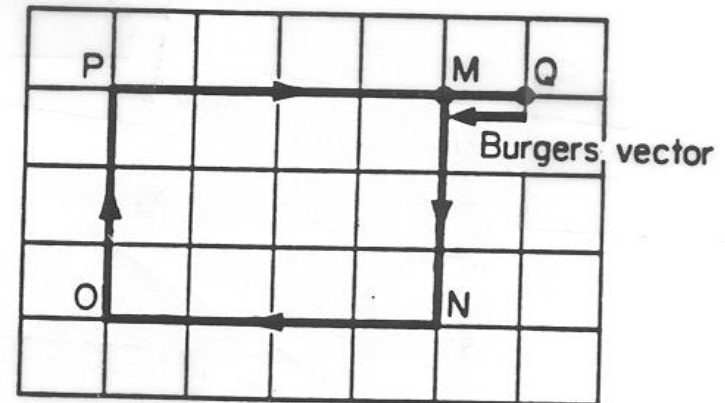
What is Burgers vector?

To determine the Burgers vector of a dislocation in a two-dimensional primitive square lattice, proceed as follows:

Trace around the end of the dislocation plane to form a closed loop. Record the number of lattice vectors travelled along each side of the loop (shown here by the numbers in the boxes):



In a perfect lattice, trace out the same path, moving the same number of lattice vectors along each direction as before. This loop will not be complete, and the closure failure is the Burgers vector:

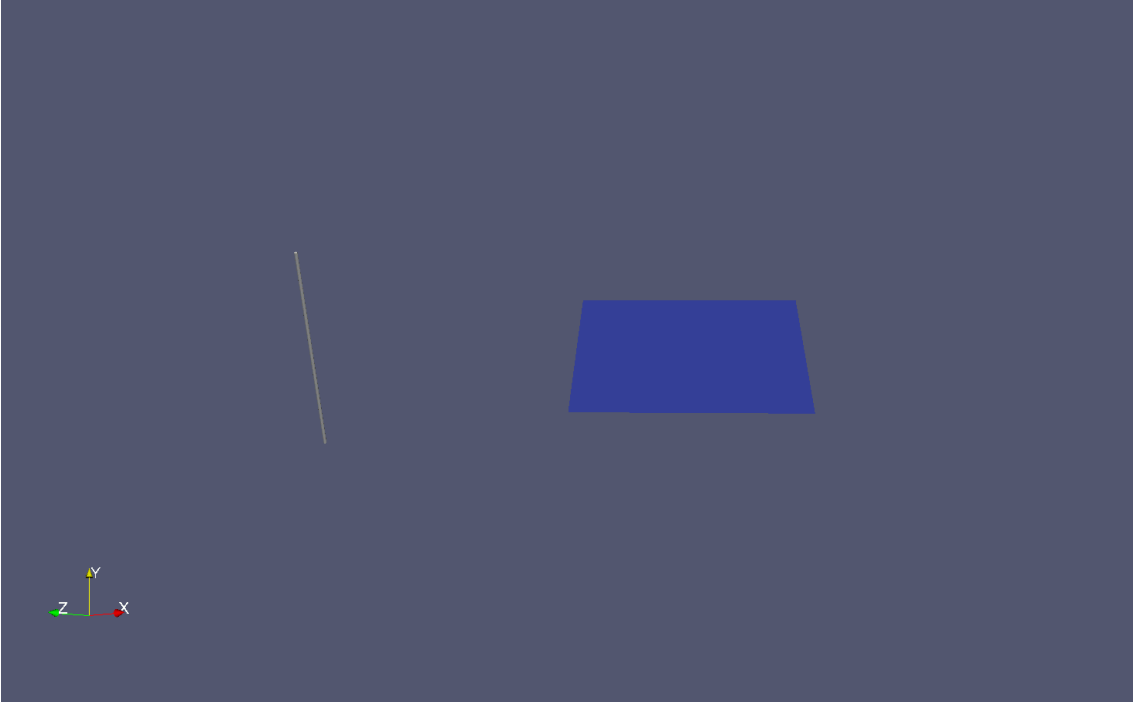
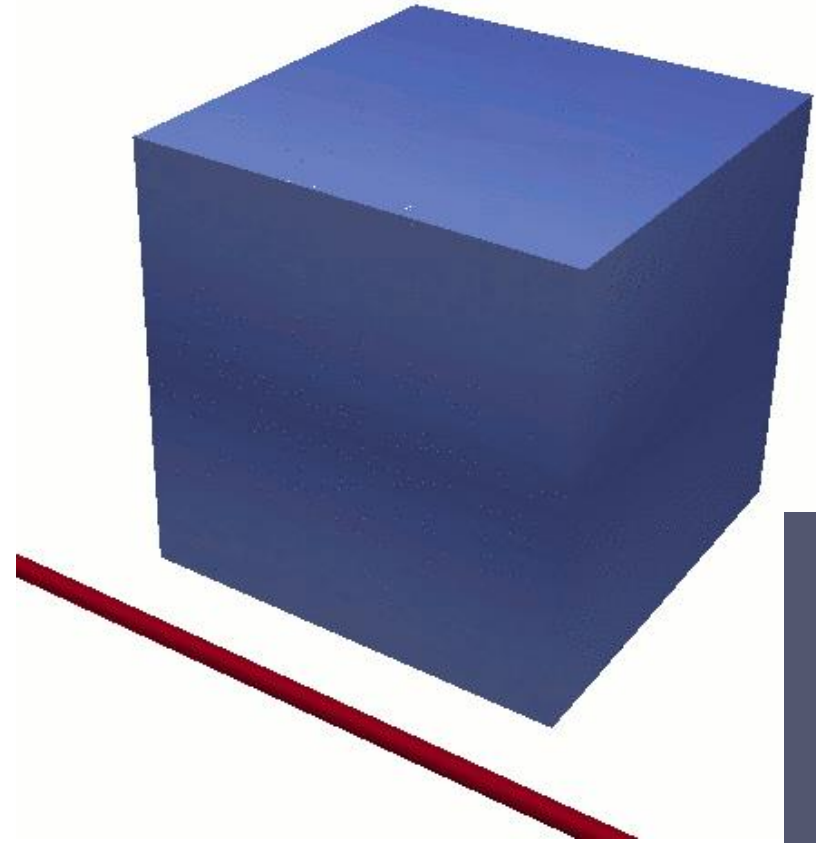


RHFS:

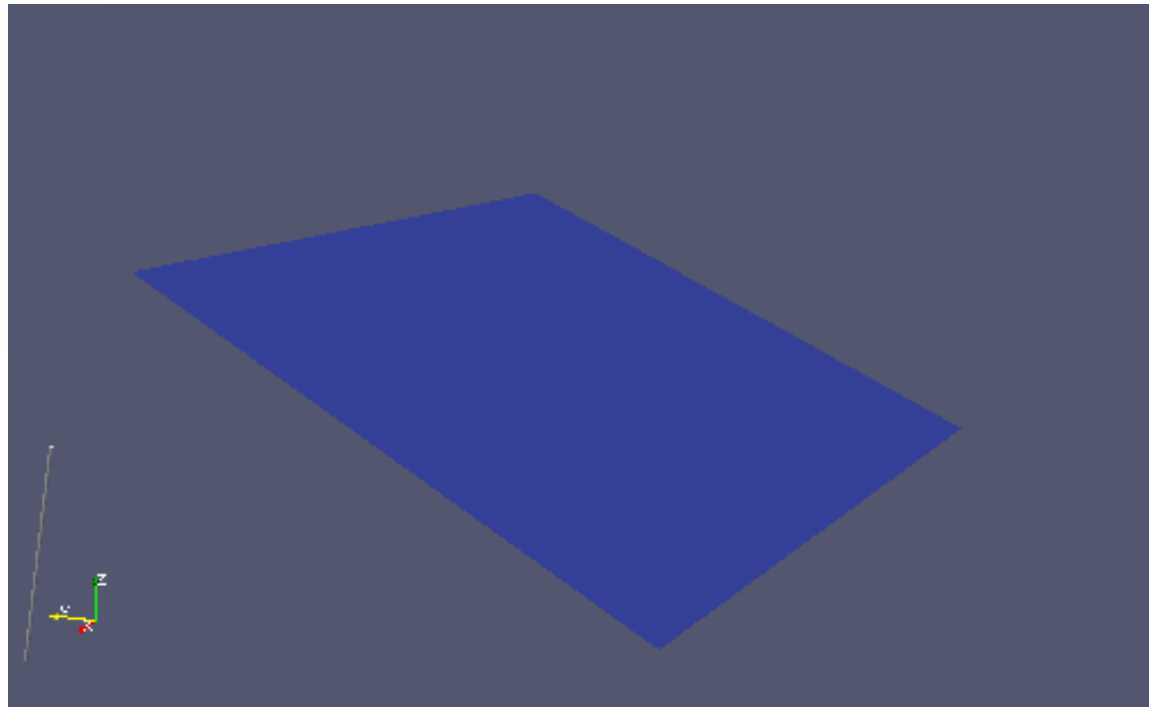
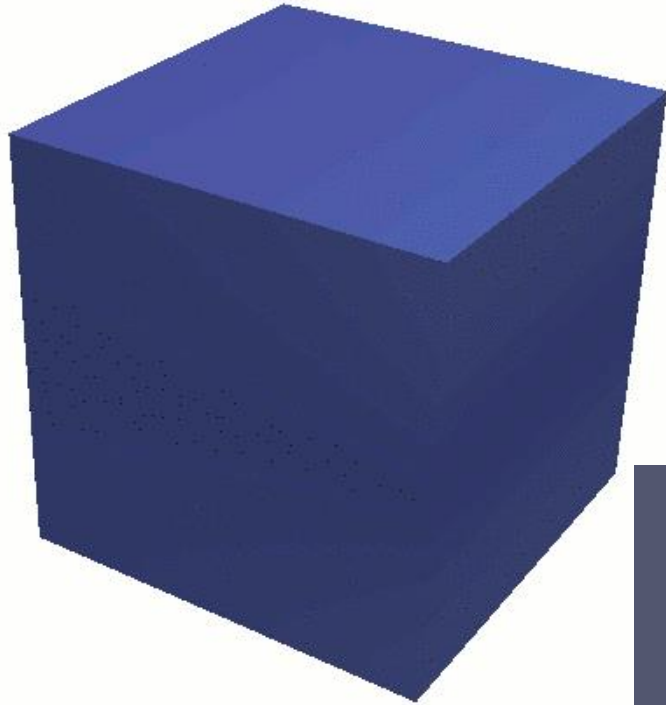
Right Hand Finish to Start
convention

Home work: Burgers vector for fcc, bcc and hcp

Movement of edge dislocation

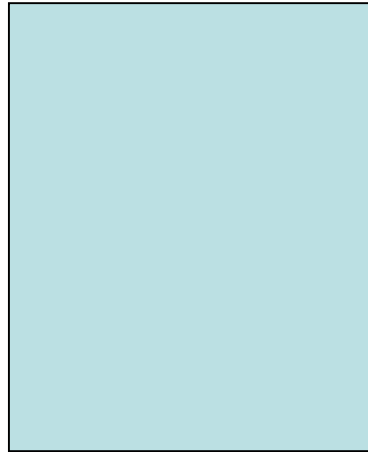


Movement of screw dislocation

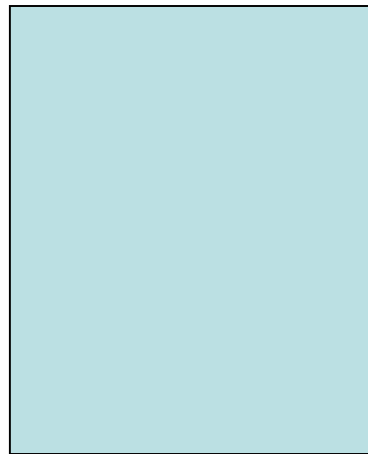


Home work: Differentiation of $\frac{\partial \tan^{-1} \frac{y}{x}}{\partial x}$ and $\frac{\partial \tan^{-1} \frac{y}{x}}{\partial y}$

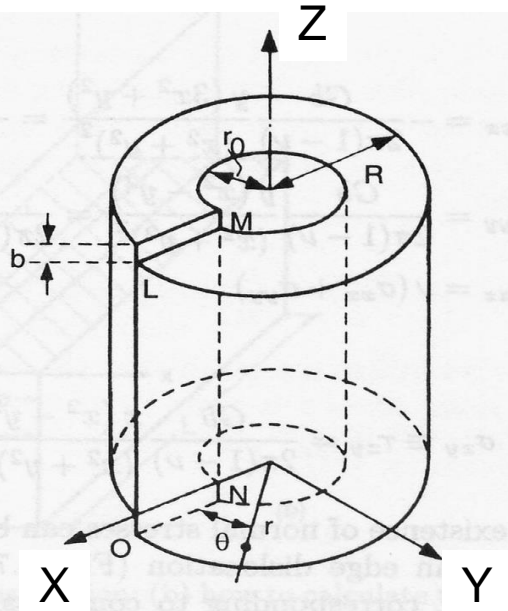
$$\frac{\partial \tan^{-1} \frac{y}{x}}{\partial x} = \frac{-\frac{y}{x^2}}{1 + \left(\frac{y}{x}\right)^2}$$



$$\frac{\partial \tan^{-1} \frac{y}{x}}{\partial y} = \frac{\frac{1}{x}}{1 + \left(\frac{y}{x}\right)^2}$$



Stress field of a screw dislocation



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

$$\epsilon_{ij} = \begin{pmatrix} 0 & 0 & \epsilon_{xz} \\ 0 & 0 & \epsilon_{yz} \\ \epsilon_{xz} & \epsilon_{yz} & 0 \end{pmatrix}$$

$$\epsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

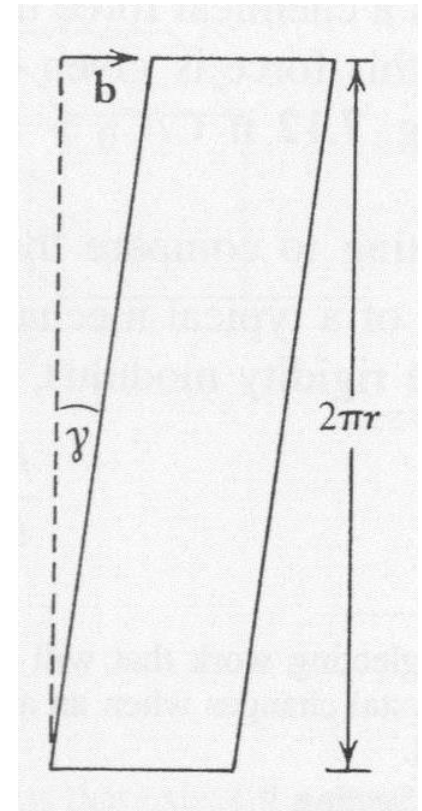
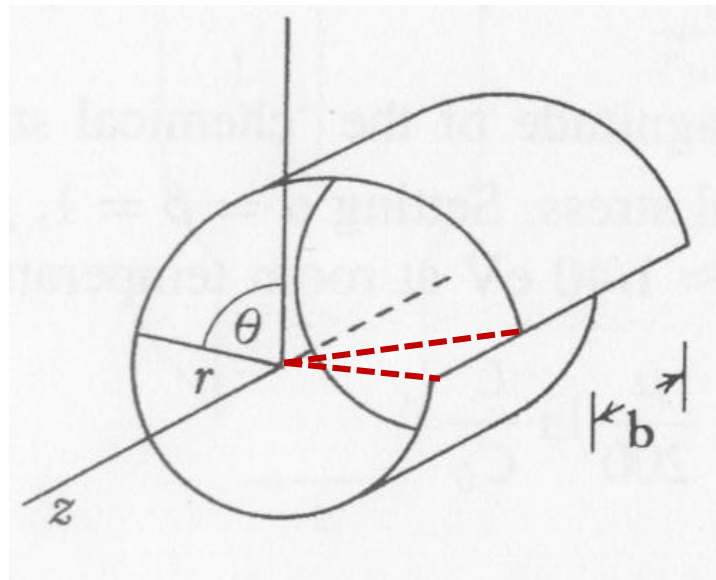
$$\epsilon_{zz} = \frac{1}{2} \frac{\partial u_z}{\partial z} = 0$$

$$\epsilon_{xx} = \epsilon_{yy} = \epsilon_{xy} = 0$$

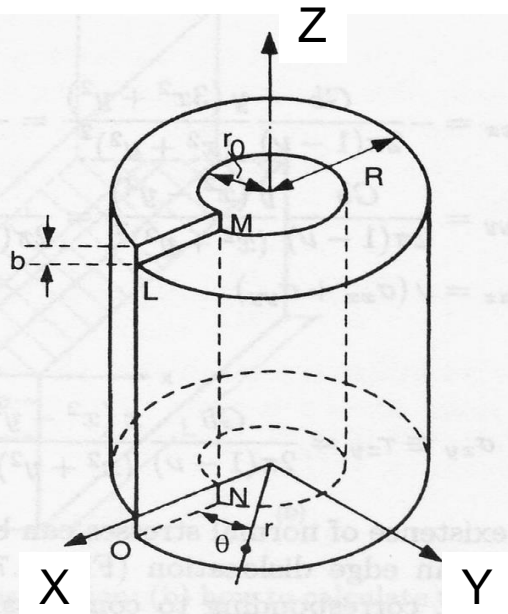
$$u_x = u = 0$$

$$u_y = v = 0$$

$$u_z = w \neq 0$$



Stress field of a screw dislocation



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

$$\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

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

$$\varepsilon_{yz} = \frac{1}{2} \frac{\partial u_z}{\partial y} = \frac{bx}{4\pi(x^2 + y^2)}$$

$$\varepsilon_{xz} = \frac{1}{2} \frac{\partial u_z}{\partial x} = -\frac{by}{4\pi(x^2 + y^2)}$$

$$\varepsilon_{zz} = \frac{1}{2} \frac{\partial u_z}{\partial z} = 0$$

$$u_x = 0$$

$$u_y = 0$$

$$u_z \neq 0$$

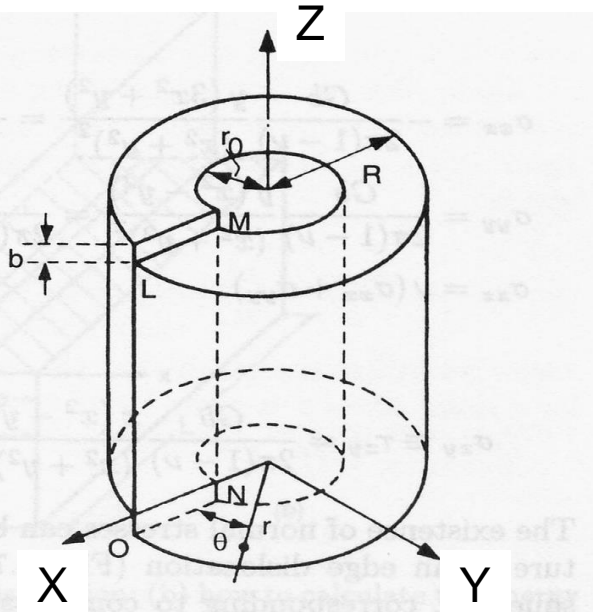
$$\sigma_{ij} = \begin{pmatrix} 0 & 0 & \sigma_{xz} \\ 0 & 0 & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & 0 \end{pmatrix}$$

$$\sigma_{yz} = \frac{Gbx}{2\pi(x^2 + y^2)}$$

$$\sigma_{xz} = \frac{-Gby}{2\pi(x^2 + y^2)}$$

Stress field of a screw dislocation

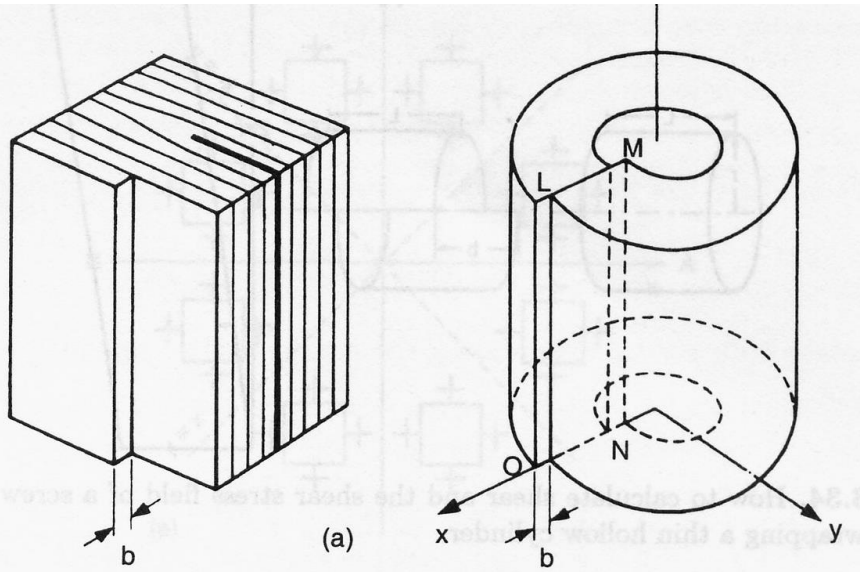
$$\sigma_{ij} = \begin{pmatrix} 0 & 0 & \sigma_{xz} \\ 0 & 0 & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & 0 \end{pmatrix}$$



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

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

Stress field of a edge dislocation



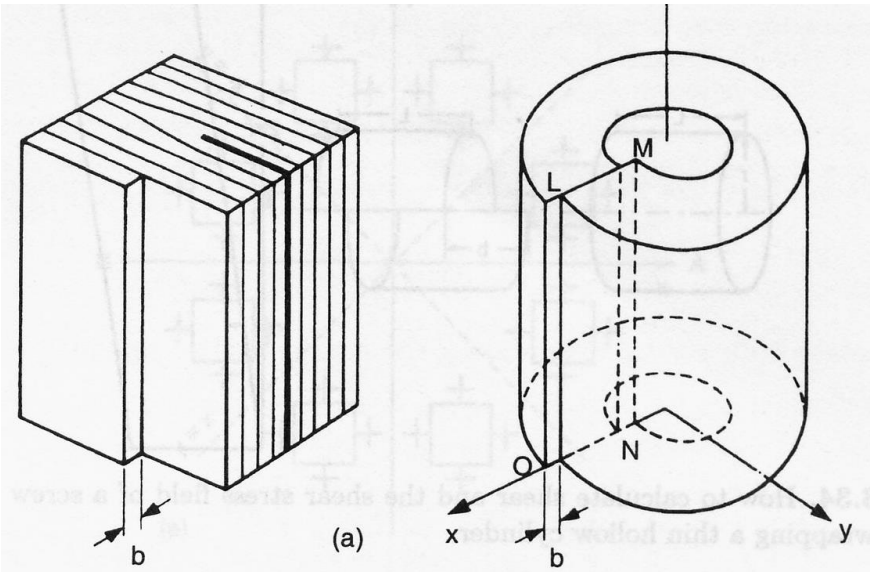
$$\sigma_{ij} = \begin{pmatrix} \sigma_{xx} & \tau_{xy} & 0 \\ \tau_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$

$$u_x = \frac{b}{2\pi} \left[\tan^{-1} \frac{y}{x} + \frac{1}{2(1-\nu)} \cdot \frac{xy}{x^2 + y^2} \right] = \frac{b}{2\pi} \left[\theta + \frac{\sin^2 \theta}{4(1-\nu)} \right]$$

$$u_y = \frac{-b}{8\pi(1-\nu)} \left[(1-2\nu) \log(x^2 + y^2) + \frac{x^2 - y^2}{x^2 + y^2} \right] = \frac{-b}{2\pi} \left[\frac{1-2\nu}{2(1-\nu)} \ln r + \frac{\cos 2\theta}{4(1-2\nu)} \right]$$

$$u_z = 0$$

Stress field of a edge dislocation



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

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

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

$$\sigma_{xy} = \sigma_{yx}$$

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

$$\sigma_{ij} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ \sigma_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$

Stress field of a edge dislocation

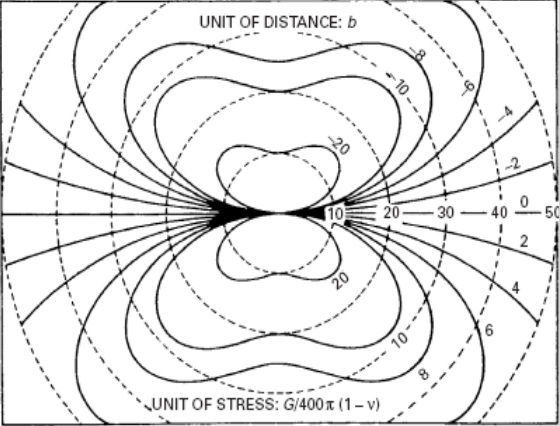
$$\sigma_{xx} = -\frac{Gb}{2\pi(1-\nu)} \frac{\sin \theta (2 + \cos 2\theta)}{r}$$

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

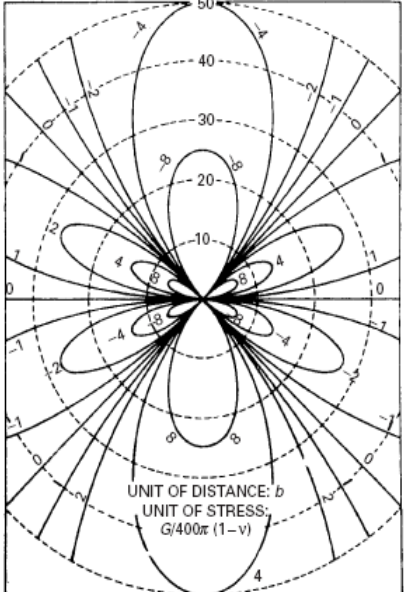
$$\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$$

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

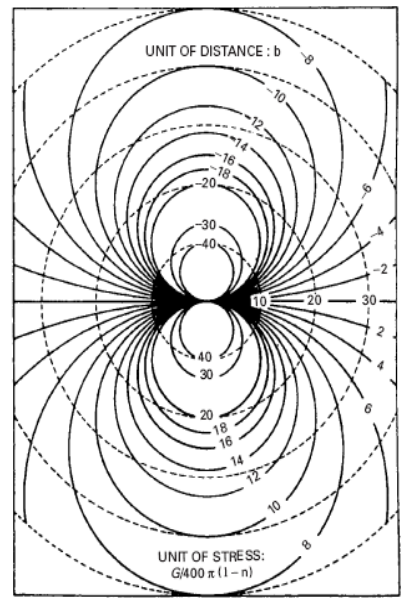
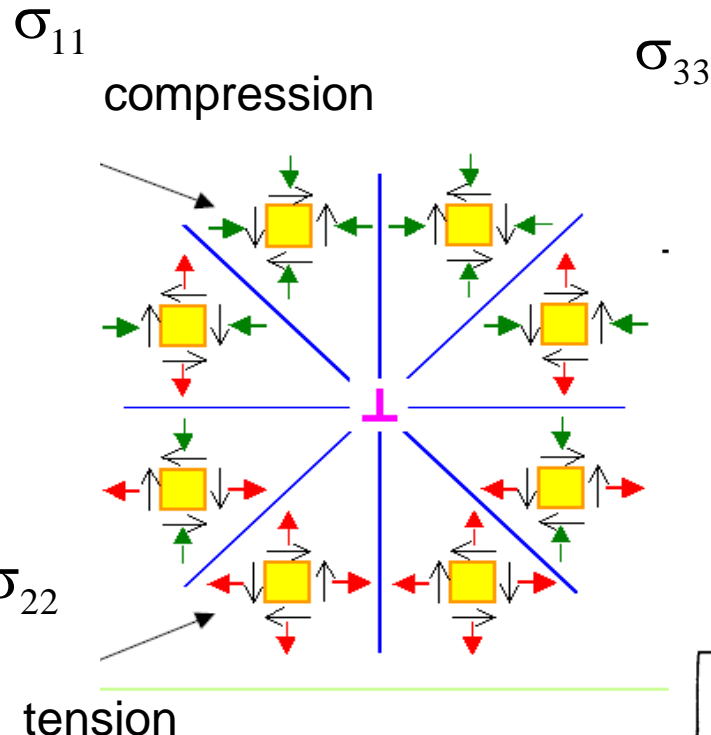
Stress Fields Around a Edge Dislocation



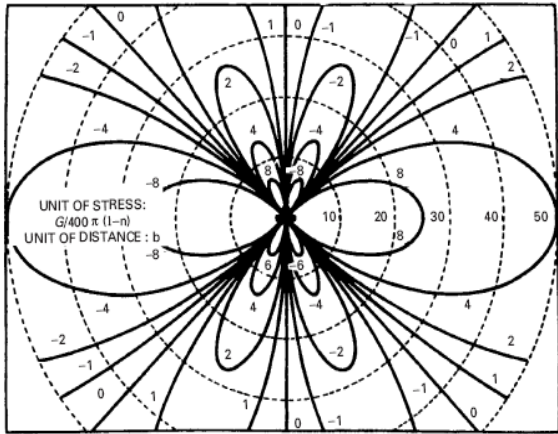
(a)



(b)



(c)



(d)

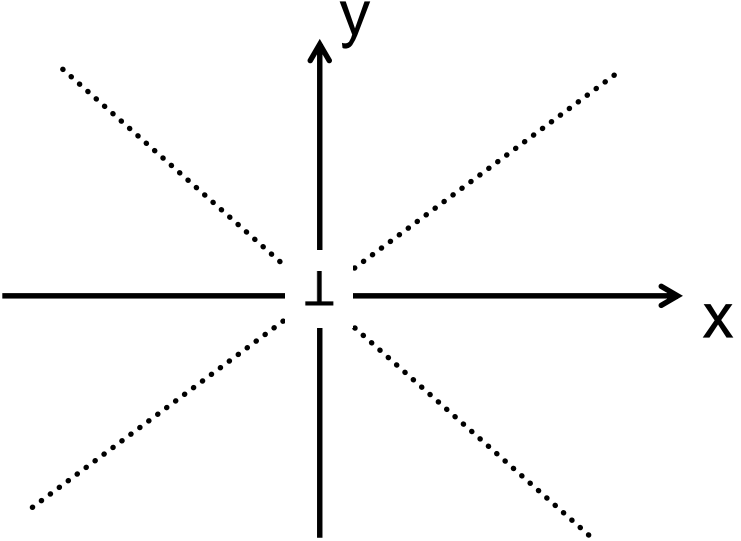
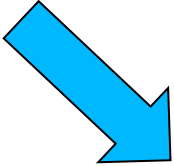
Forces on dislocations: Peach-Koehler equation

$$\vec{F}_{12} = (\sigma_1 \cdot \vec{b}_2) \times \vec{l}_2$$

$$\sigma_1 = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ \sigma_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$

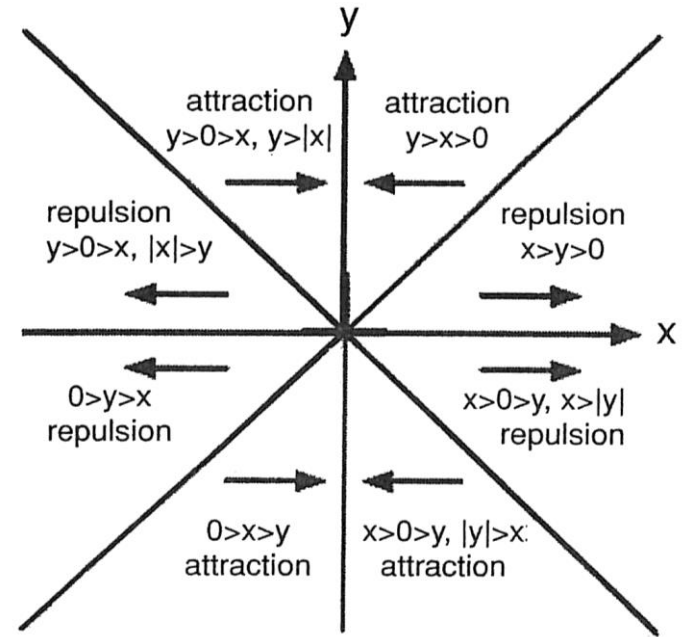
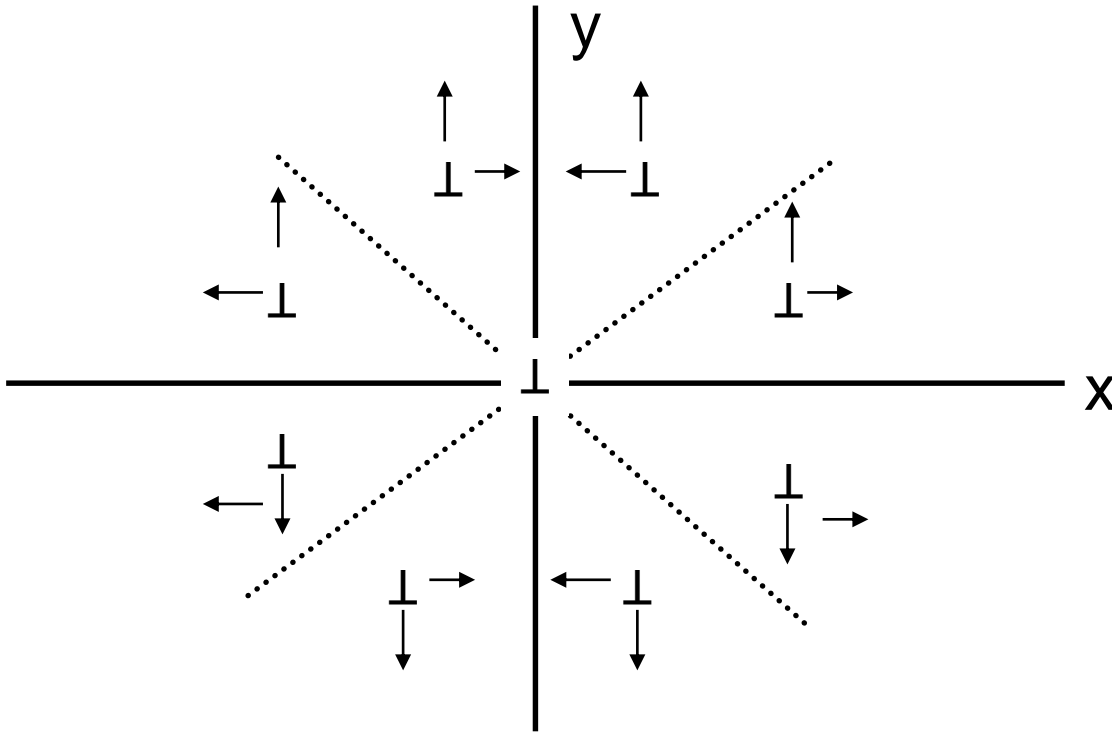
$$\vec{b}_2 = \begin{pmatrix} b \\ 0 \\ 0 \end{pmatrix}$$

$$\vec{l}_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$



$$F = \tau b$$

Forces on dislocations: Peach-Koehler equation

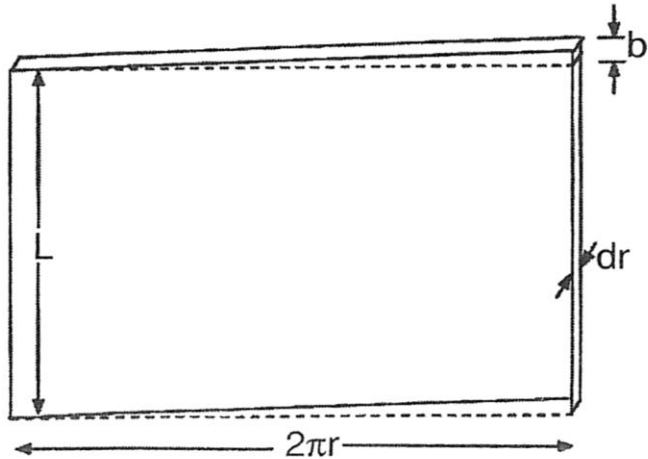
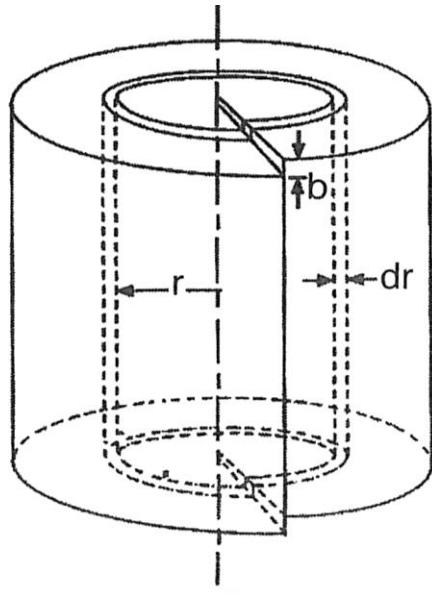


$$\vec{F}_{12} = \begin{pmatrix} \sigma_{xy} b_2 \\ -\sigma_{xx} b_2 \\ 0 \end{pmatrix}$$

$$\sigma_{xy} = \frac{Gb_1 b_2}{2\pi(1-\nu)} \frac{x(x^2 - y^2)}{(x^2 + y^2)^2}$$

$$\sigma_{xx} = -\frac{Gb_1 b_2}{2\pi(1-\nu)} \frac{y(3x^2 + y^2)}{(3x^2 + y^2)^2}$$

Energy of screw dislocation



$$\tau_{\theta z} = G\gamma$$
$$\gamma = \frac{b}{2\pi r}$$
$$E_v = \frac{1}{2} \tau_{\theta z} \gamma$$

$$E_v = \frac{G\gamma^2}{2}$$

$$E_v = \frac{Gb^2}{8\pi^2 r^2}$$

Energy of screw dislocation

$$E_{\text{screw}} = \int_0^{2\pi} \int_{r_0}^r \frac{Gb^2}{8\pi^2 r^2} \cdot r dr d\theta \cdot l$$

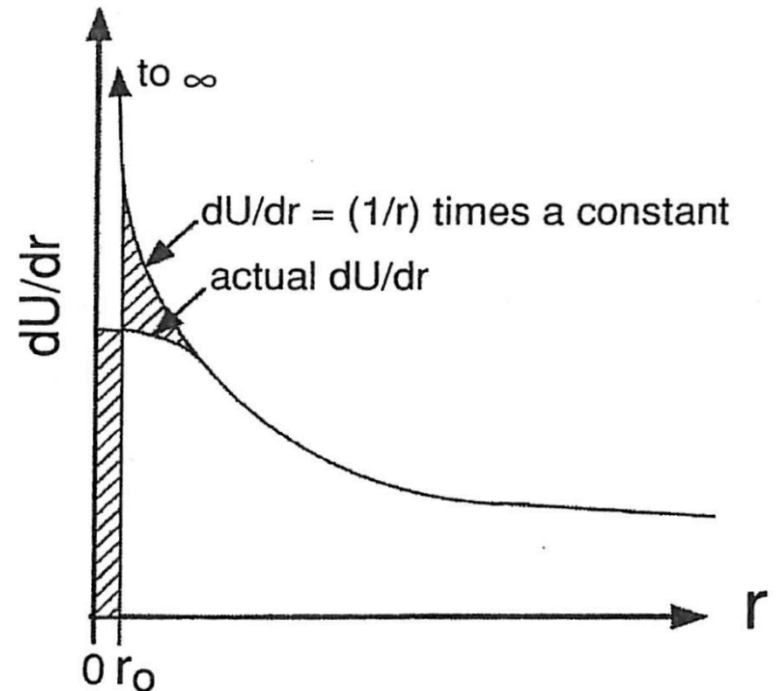
$$= l \cdot \frac{Gb^2}{4\pi} \ln\left(\frac{r}{r_0}\right)$$

$$\frac{E_{\text{screw}}}{l} = \frac{Gb^2}{4\pi} \ln\left(\frac{r}{r_0}\right)$$

$$\frac{E_{\text{edge}}}{l} = \frac{Gb^2}{4\pi(1-\nu)} \ln\left(\frac{r}{r_0}\right)$$

$$\frac{E_{\text{dis}}}{l} \approx \frac{1}{2} Gb^2$$

The strain energy per unit length in order to obtain minimum energy, that is, to possess a line tension analogous to the surface tension.



Partial dislocations in fcc

FCC

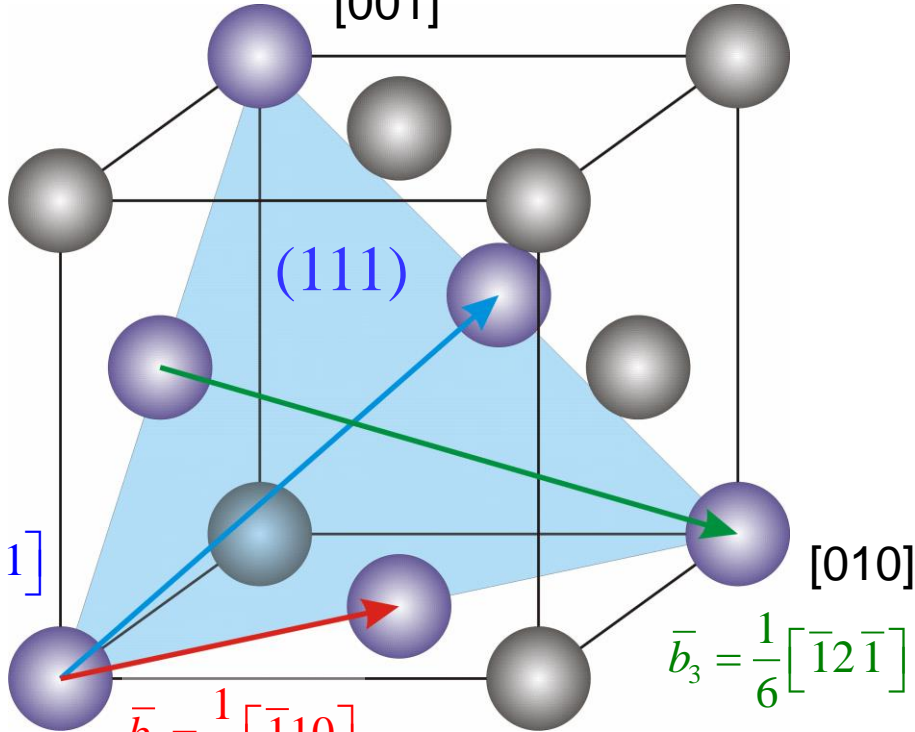
(111)
Slip plane

$$\bar{b}_2 = \frac{1}{6}[\bar{2}11]$$

[100]

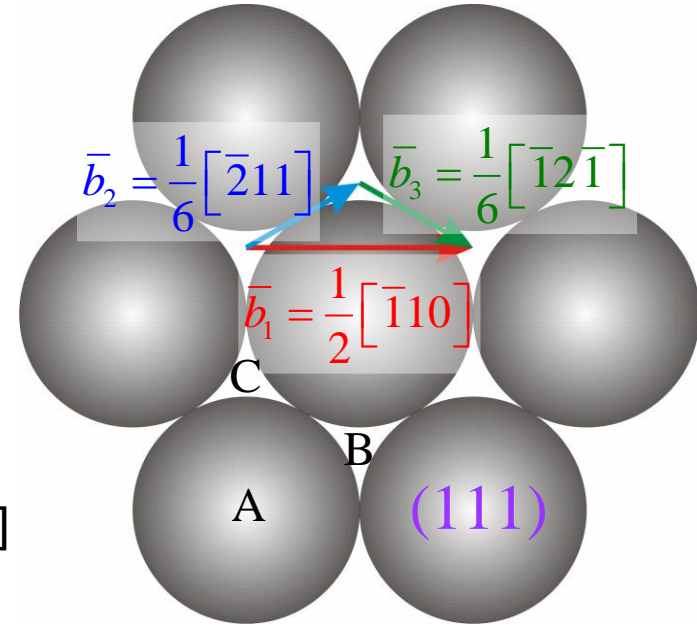
$$\bar{b}_1 = \frac{1}{2}[\bar{1}10]$$

[001]



$$\bar{b}_3 = \frac{1}{6}[\bar{1}2\bar{1}]$$

Some of the atoms are omitted for clarity



$$\left(\frac{1}{2}[\bar{1}10] \right)_{(111)}$$

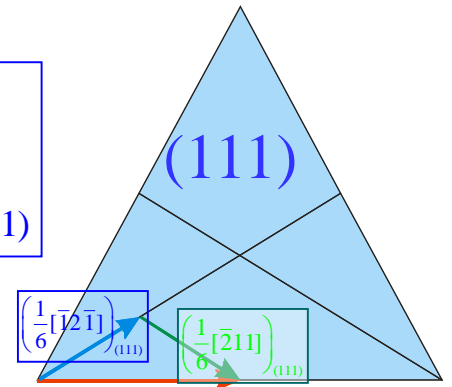


$$\left(\frac{1}{6}[\bar{1}2\bar{1}] \right)_{(111)}$$

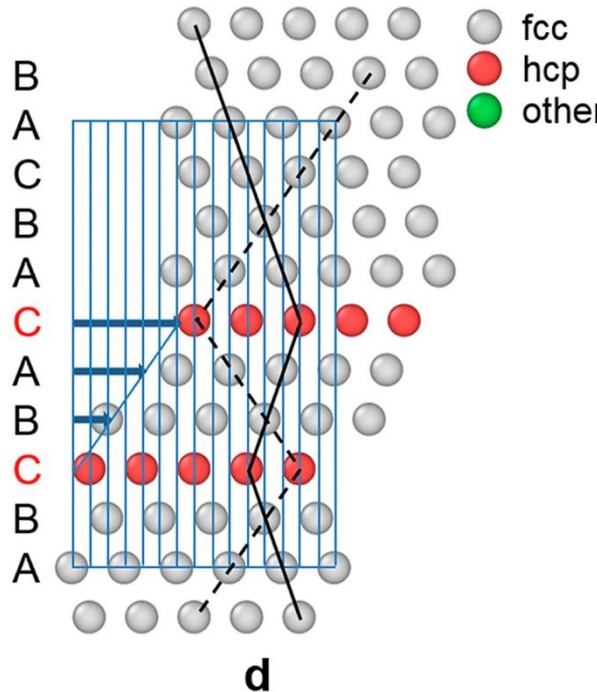
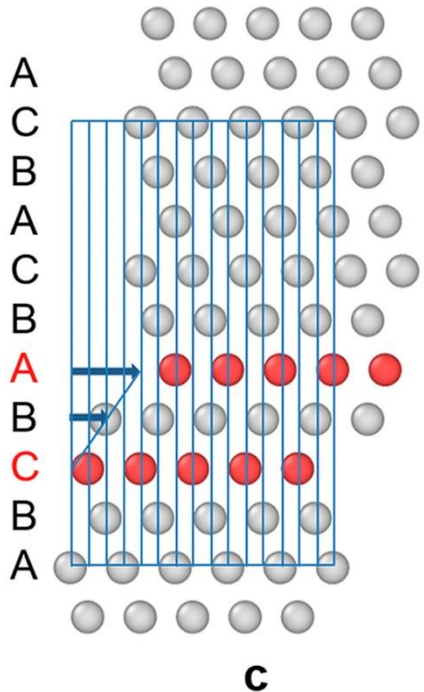
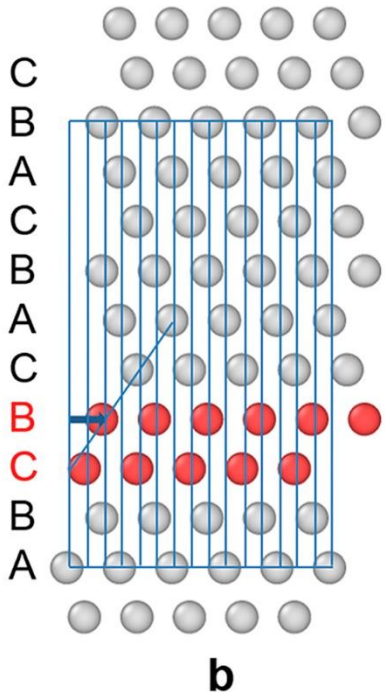
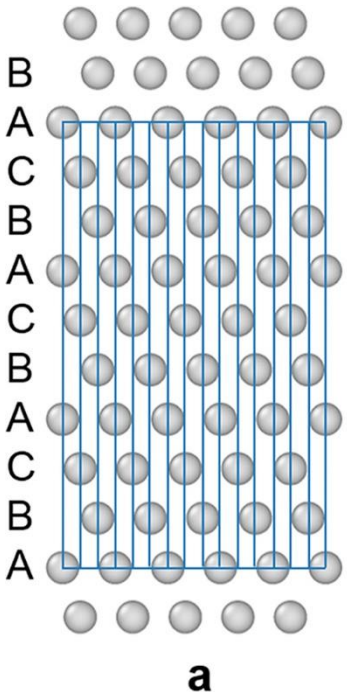
+

$$\left(\frac{1}{6}[\bar{2}11] \right)_{(111)}$$

Shockley Partials

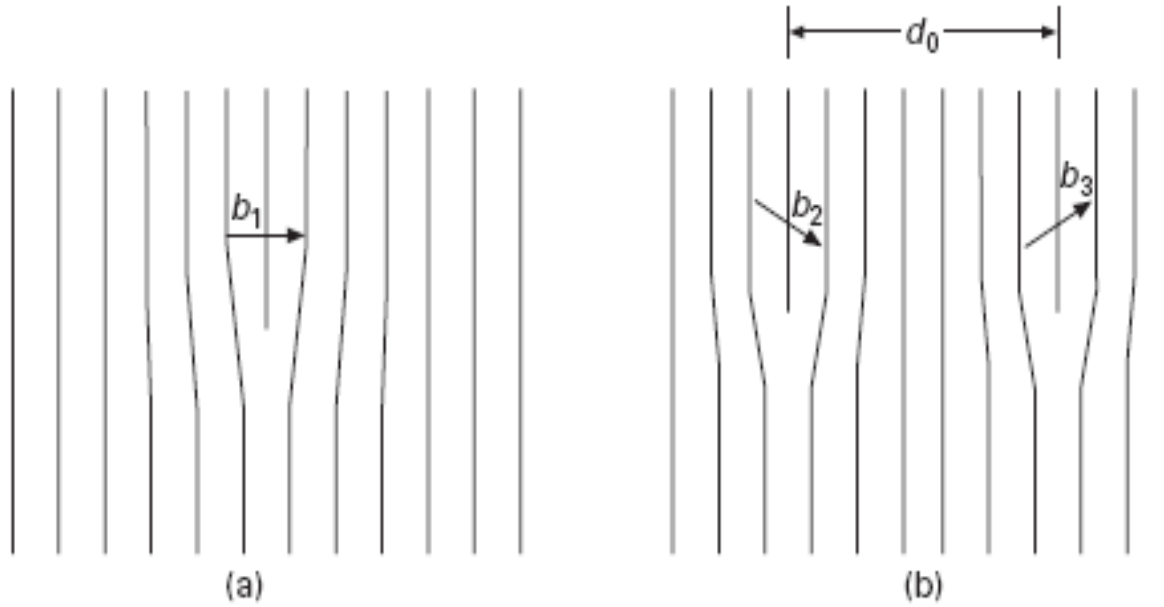


Dislocations and Stacking faults



● fcc
● hcp
● other

Partial dislocations



$$U_L \approx Gb^2$$

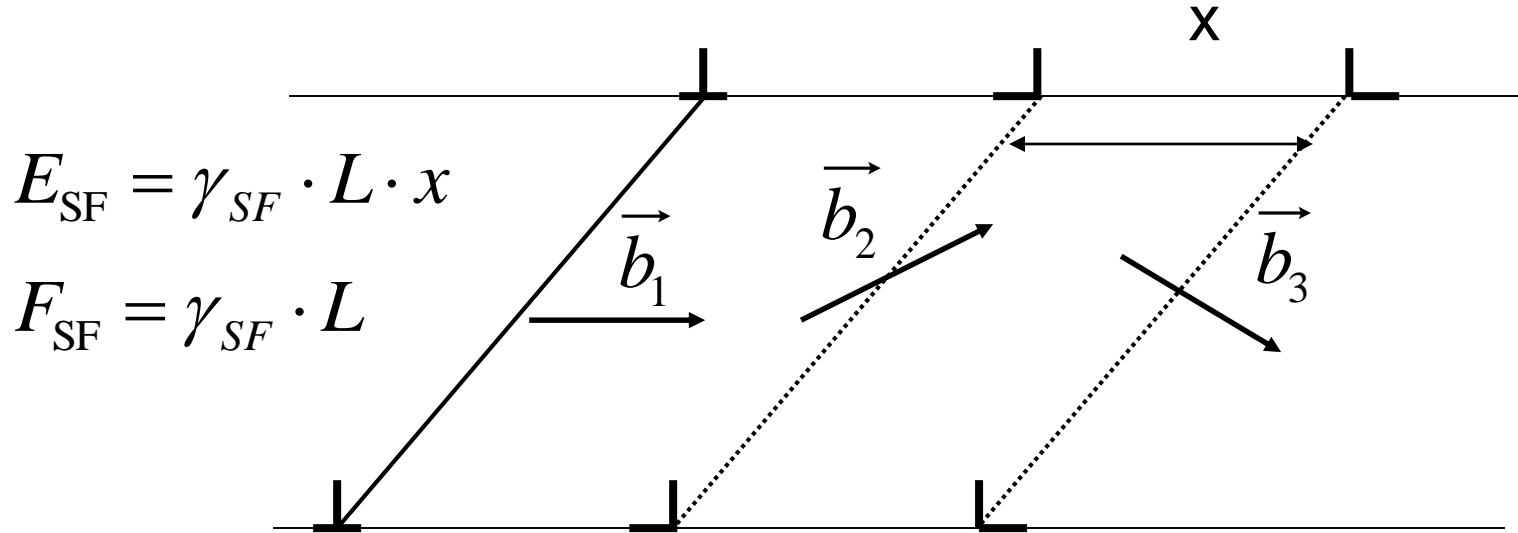
$$U_L = \frac{1}{2}Gb_1^2 \quad \gg \quad U_L = \frac{1}{2}(Gb_2^2 + Gb_3^2)$$

Stacking faults in fcc

Table 9.2. Stacking fault energies of several fcc metals

Ag	Al	Au	Cu	Ni	Pd	Pt	Rh	Ir
16	166	32	45	125	180	322	750	300 mJ/m ² .

Source From listing in J. P. Hirth and J. Lothe, *Theory of Dislocations*, Wiley, (1982).



Stacking faults energy

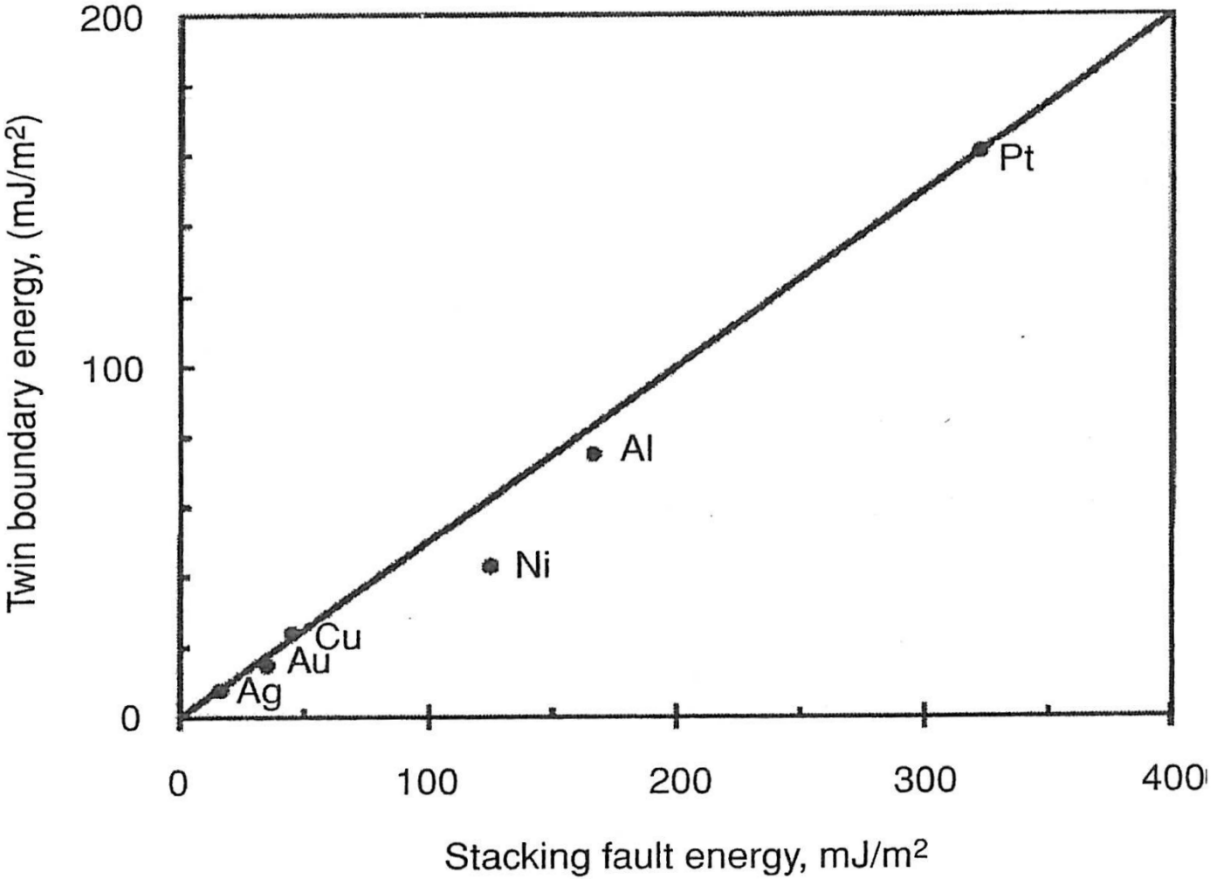


Figure 9.24. The relationship of stacking fault energy and twin boundary energy. The line represents $\gamma_{\text{stacking fault}} = 2\gamma_{\text{twin}}$.

References:

1. A. Kelly, G.W. Groves and P. Kidd, "Crystallography and crystal defects", revised edition, 2000, John Wiley & Sons Ltd., England.
2. G. Gottstein, "Physical Foundations of Materials Science", 2004, Springer Verlag, Heidelberg.