



Physics of Materials

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Chapter 7: Elasticity Theory of Dislocations



Masters Course PHYS-307

Fall 2024

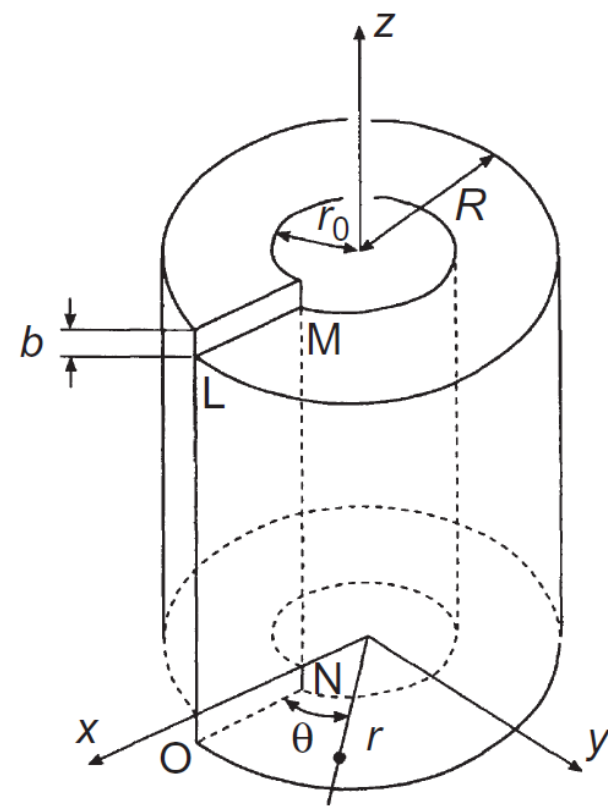
Stress field around a (screw) dislocation

1) Equilibrium (Navier-Stokes) equation

$$(1 - 2\nu)\Delta\vec{u} + \overrightarrow{\text{grad}}(\text{div}(\vec{u})) = 0$$

2) Conservation of $\vec{b} = \oint \frac{\partial \vec{u}}{\partial x} dx$

3) The exterior surfaces are free of any force or torque



Screw dislocation

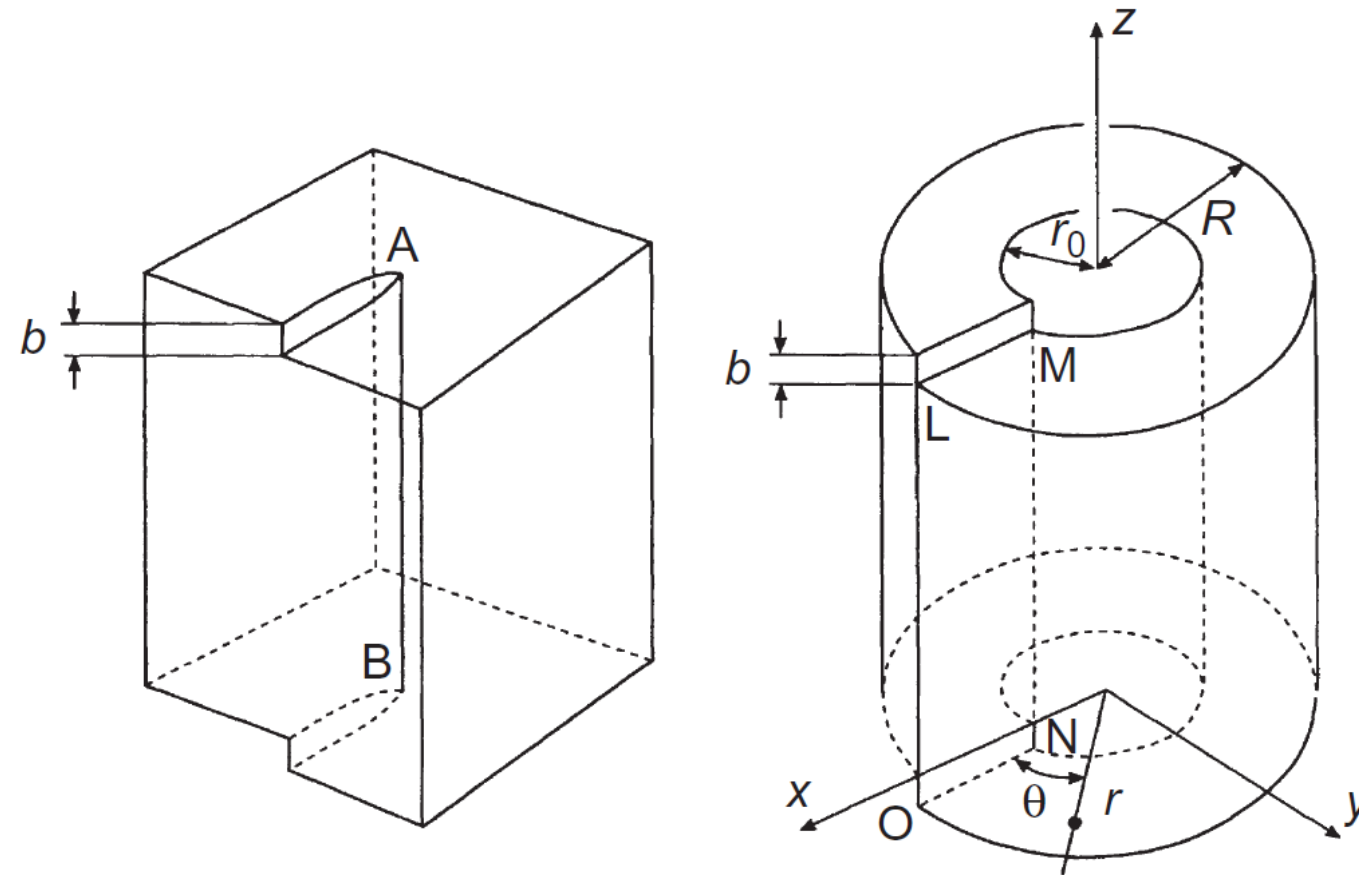
$$\sigma_{ij} dS_j = 0$$

$$u_r = u_\theta = 0 \quad u_z = \frac{b\theta}{2\pi}$$

$$u_{\theta z} = u_{z\theta} = \frac{1}{2} \left(\frac{\partial u_\theta}{\partial z} + \frac{\partial u_z}{r \partial \theta} \right) = \frac{b}{4\pi r}$$

$$\sigma_{\theta z} = \sigma_{z\theta} = 2\mu u_{\theta z} = \frac{\mu b}{2\pi r}$$

Stress field around a (screw) dislocation

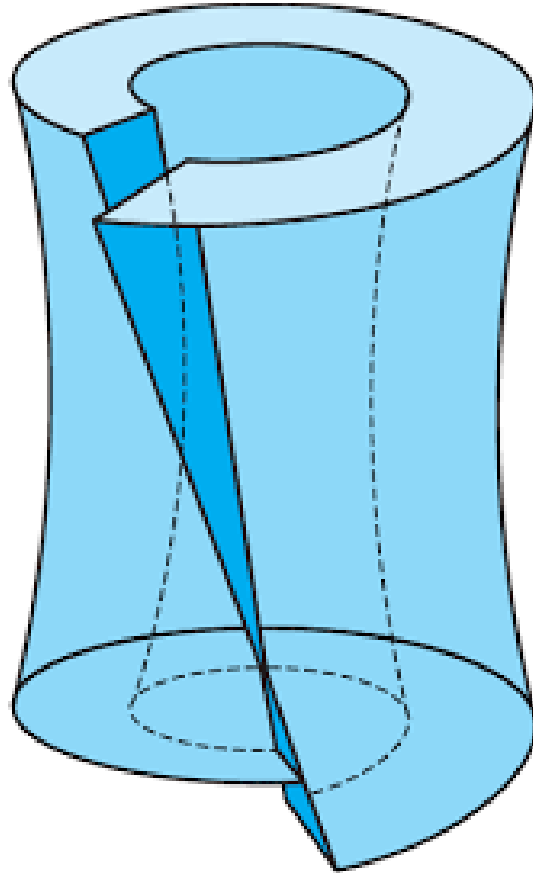


In cartesian coordinates

$$\sigma_{xz} = 2\mu u_{xz} = -\frac{\mu b}{2\pi} \frac{y}{x^2 + y^2}$$

$$\sigma_{yz} = 2\mu u_{yz} = \frac{\mu b}{2\pi} \frac{x}{x^2 + y^2}$$

Screw dislocation (finite length)



The previous solution is valid for an infinite medium:

non-zero stress at the surface

$$M_z = \int_0^{2\pi} \int_{r_0}^R r \sigma_{\theta z} r dr d\theta = \mu b \int_{r_0}^R r dr = \frac{\mu b}{2} (R^2 - r_0^2)$$

We suppose the presence of a counter-torque

$$M'_z = -\frac{\mu b}{2} (R^2 - r_0^2)$$

$$u'_\theta = -r\varphi(z) = -Arz$$

$$u'_{z\theta} = -\frac{Ar}{2} \quad \sigma'_{z\theta} = -\mu Ar$$

$$M'_z = -\int_0^{2\pi} \int_{r_0}^R r \sigma'_{\theta z} r dr d\theta = -2\pi\mu A \int_{r_0}^R r^3 dr = -\frac{\pi\mu A}{2} (R^4 - r_0^4)$$

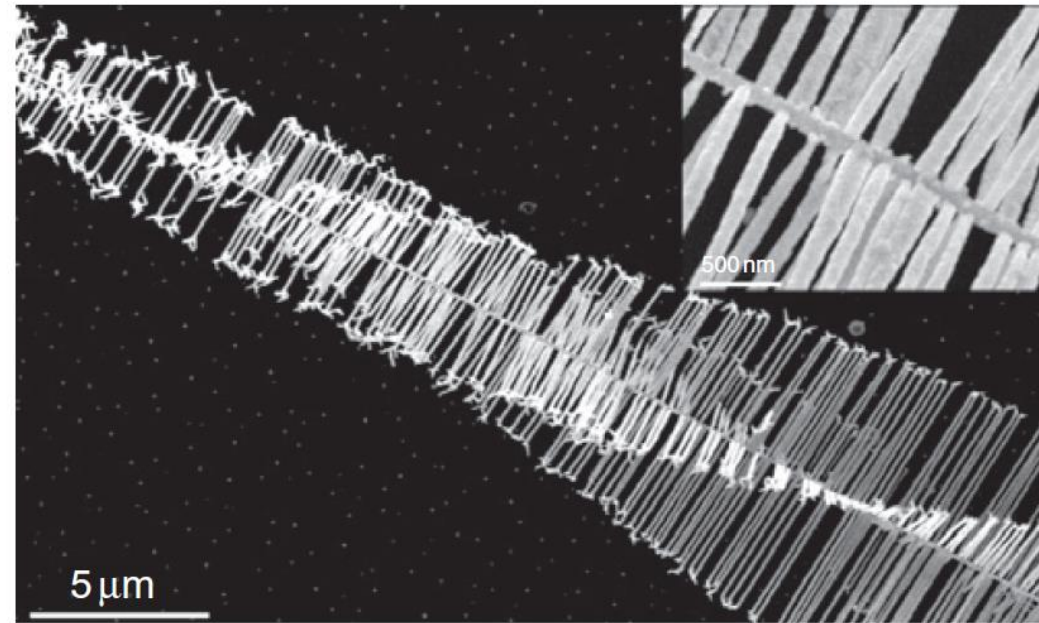
$$M'_z = -M_z \rightarrow A = \frac{b}{\pi} \frac{R^2 - r_0^2}{R^4 - r_0^4}$$

solution

$$u_{\theta z} = \frac{b}{4\pi r} \left(1 - \frac{2r^2}{R^2} \right)$$

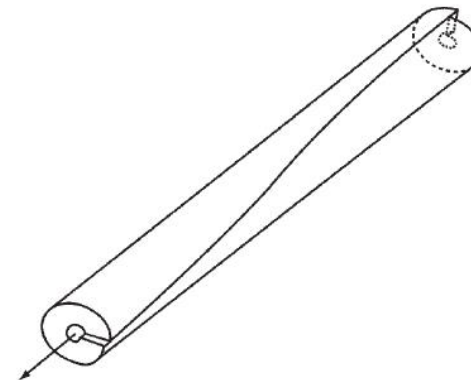
$$\sigma_{\theta z} = \frac{\mu b}{2\pi r} \left(1 - \frac{2r^2}{R^2} \right)$$

Screw dislocation and Eshelby twist

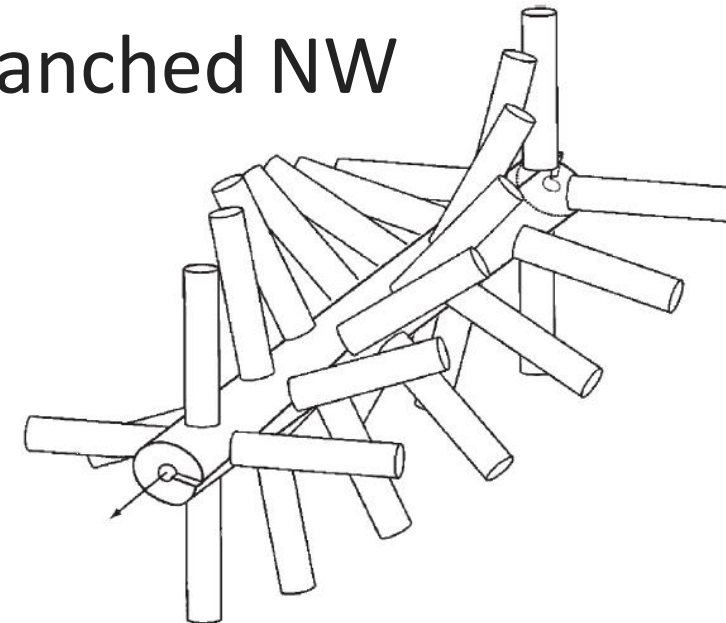


(a)

PbSe chiral branched NW



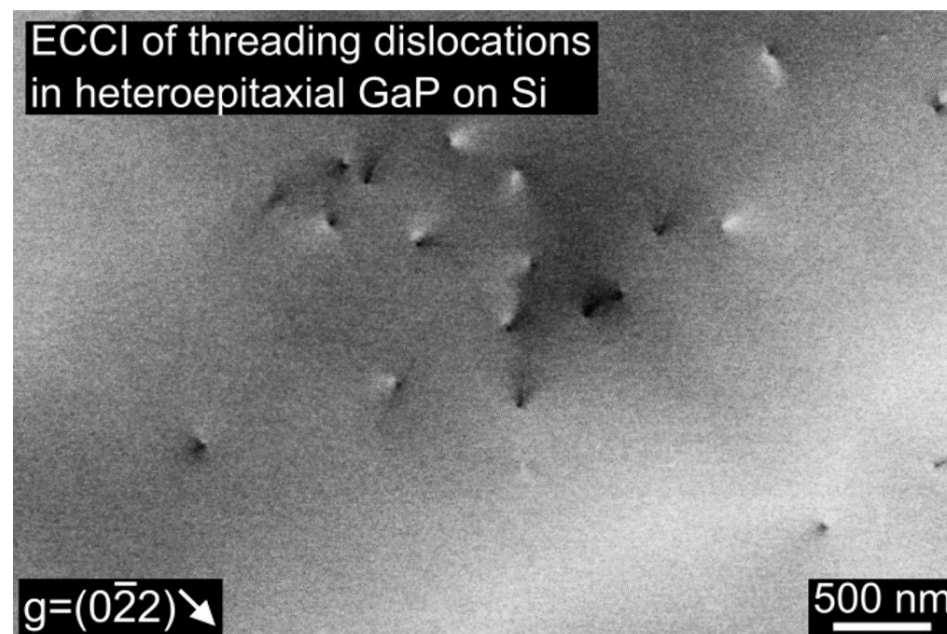
(b)



(c)

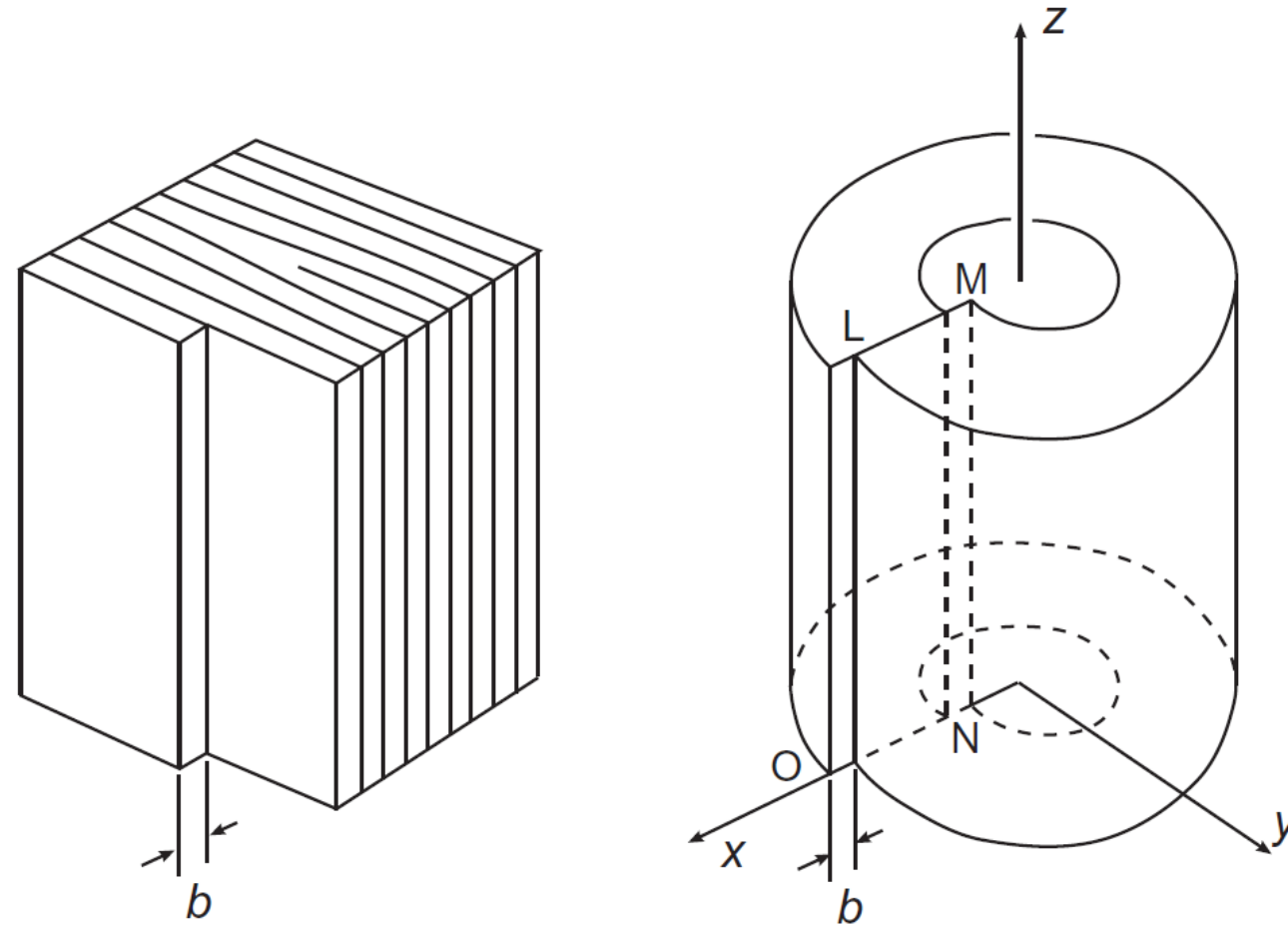
$$\sigma_{\theta z} = \frac{\mu b}{2\pi r} \left(1 - \frac{2r^2}{R^2} \right)$$

This stress results in a torque that twists the crystal about the screw dislocation.



This twist of the crystal results in a distortion on the crystal surface, and you can detect subsurface dislocations in thin films using electron channeling contrast imaging (ECCL) in the scanning electron microscope.

Edge dislocation (finite length)



$$u_x = \frac{b}{2\pi} \left(\theta + \frac{\sin 2\theta}{4(1-\nu)} \right)$$

$$u_y = -\frac{b}{2\pi} \left(\frac{1-2\nu}{2(1-\nu)} \ln r + \frac{\cos 2\theta}{4(1-\nu)} \right)$$

Edge dislocation stress tensor

The application of the Hooke law allows to calculate the stress tensor

$$\sigma_{xx} = -D \frac{\sin \theta (2 + \cos 2\theta)}{r} \quad \sigma_{xy} = D \frac{\cos \theta \cos 2\theta}{r} \quad \sigma_{yy} = D \frac{\sin \theta \cos 2\theta}{r}$$

$$\sigma_{zz} = -2\nu D \frac{\sin \theta}{r} \quad \sigma_{xz} = \sigma_{zx} = \sigma_{yz} = \sigma_{zy} = 0 \quad D = \frac{\mu b}{2\pi(1-\nu)}$$

Cylindrical Coordinates

$$\sigma_{rr} = \sigma_{\theta\theta} = -D \frac{\sin \theta}{r} \quad u_{rr} = u_{\theta\theta} = \frac{D(1-2\nu)}{2\mu} \frac{\sin \theta}{r}$$

$$\sigma_{r\theta} = D \frac{\cos \theta}{r} \quad u_{r\theta} = -\frac{D}{2\mu} \frac{\cos \theta}{r}$$

$$\sigma_{zz} = -2D\nu \frac{\sin \theta}{r} \quad u_{zz} = u_{\theta z} = u_{rz} = 0$$

Cartesian Coordinates

$$\sigma_{xx} = -D\gamma \frac{(3x^2 + y^2)}{(x^2 + y^2)^2}$$

$$\sigma_{yy} = D\gamma \frac{(x^2 - y^2)}{(x^2 + y^2)^2}$$

$$\sigma_{xy} = \sigma_{yx} = Dx \frac{(x^2 - y^2)}{(x^2 + y^2)^2}$$

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

Elastic energy

$$E_{total} = E_{core} + E_{elastic strain}$$

$$W = \frac{1}{2} \int \sigma_{ij} u_{ij} dV$$

$$w = \frac{1}{2} (\sigma_{\theta z} u_{\theta z} + \sigma_{z\theta} u_{z\theta}) = \frac{\mu b^2}{8\pi r^2} \left(1 - \frac{2r^2}{R^2} \right)^2$$

$$W = \int_0^1 dz \int_0^{2\pi} d\theta \int_{r_0}^R w r dr = \int_{r_0}^R \frac{\mu b^2}{4\pi r} \left(1 - \frac{2r^2}{R^2} \right)^2 dr \quad W = \frac{\mu b^2}{4\pi} \left[\ln r - 2 \frac{r^2}{R^2} + \frac{r^4}{R^4} \right]_{r_0}^R$$

$$W \approx \frac{\mu b^2}{4\pi} \left(\ln \frac{R}{r_0} - 1 \right)$$

Edge dislocation

Screw dislocation (infinite)

Mixed dislocation

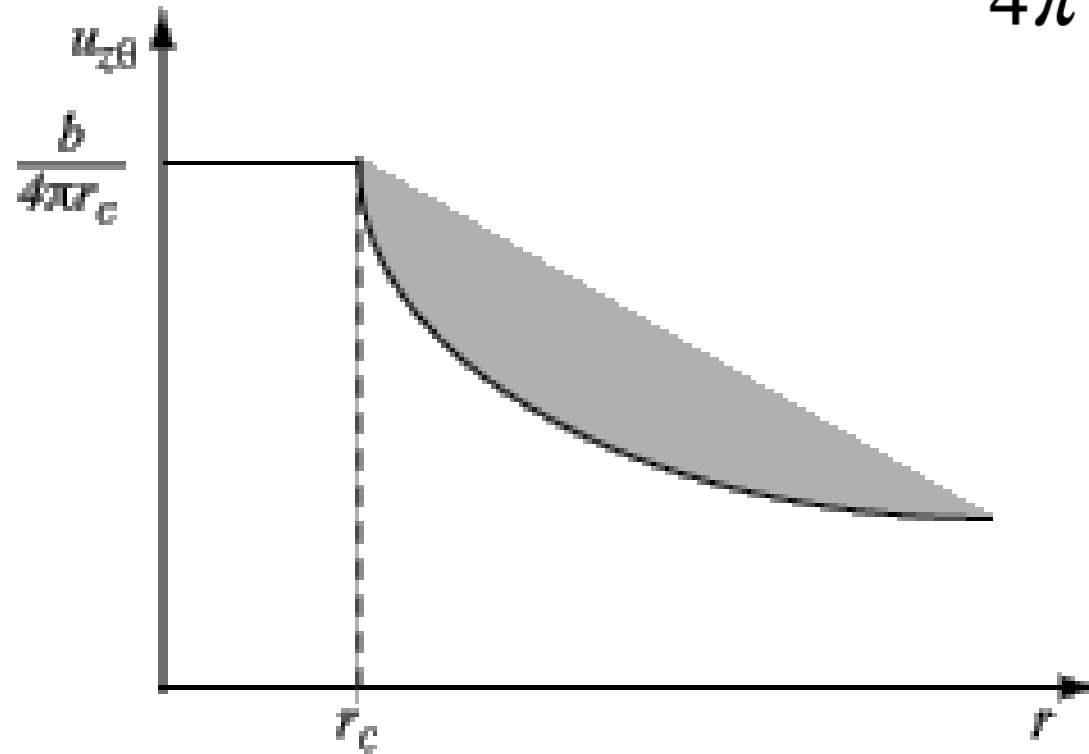
$$W \approx \frac{\mu b^2}{4\pi(1-\nu)} \ln \frac{R}{r_0}$$

$$W \approx \frac{\mu b^2}{4\pi} \ln \frac{R}{r_0}$$

$$W \approx \frac{\mu b^2}{4\pi(1-\nu)} (1 - \nu \cos^2 \psi) \ln \frac{R}{r_0}$$

Core of a dislocation

$$W \approx \frac{\mu b^2}{4\pi} \ln \frac{R}{r_0} \rightarrow \infty \text{ if } r_0 \rightarrow 0$$



Filled core

$$W_0 = \frac{1}{2} (2\sigma_{z\theta} u_{z\theta}) \pi r^2 \quad \sigma_{z\theta} = 2\mu u_{\theta z} = \frac{\mu b}{2\pi r}$$

Screw dislocation

$$W_0 = \frac{\mu b^2}{8\pi^2 r_c^2} \pi r_c^2 = \frac{\mu b^2}{8\pi} \quad \text{lower limit}$$

$$\text{upper limit: melting heat } W_0 \approx \frac{\mu b^2}{5}$$

$$\text{mean } W_0 \approx \frac{\mu b^2}{5\pi}$$

$$W_t = W + W_0 = \frac{\mu b^2}{4\pi} \left(\left(\ln \frac{R}{r_c} \right) + \frac{4\pi}{5\pi} \right) = \frac{\mu b^2}{4\pi} \left(\ln \frac{R}{b} + \ln \frac{b}{r_c} + \frac{4\pi}{5\pi} \right) \simeq \frac{\mu b^2}{4\pi} \ln \frac{R}{b}$$

Hollow core

Example: Nanotubes

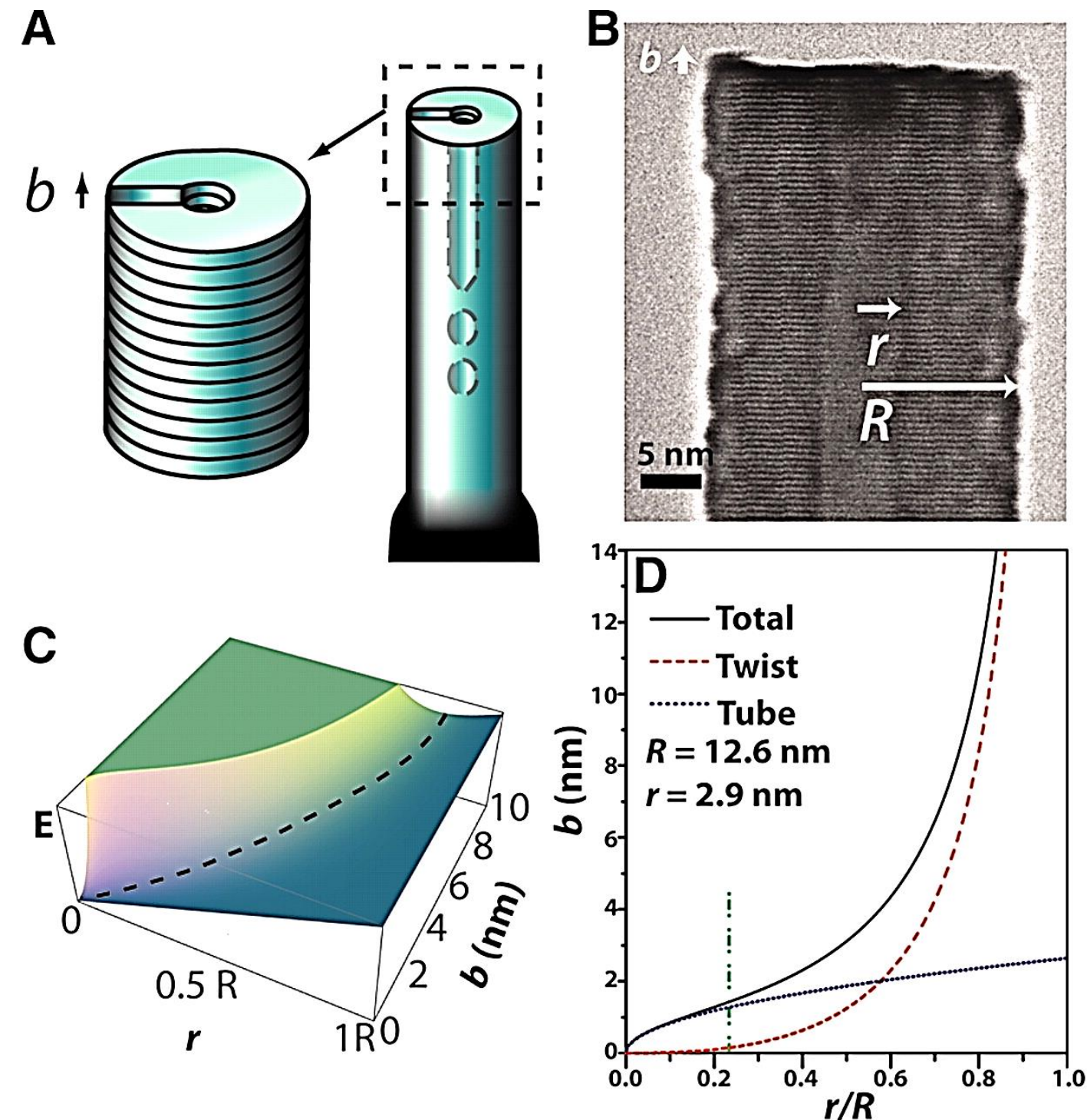
$$W \approx \frac{\mu b^2}{4\pi} \ln \frac{R}{r} + 2\pi r \gamma$$

$$\left. \frac{\partial W}{\partial r} \right|_{r=r_0} = 0 \quad r_0 = \frac{\mu b^2}{8\pi^2 \gamma}$$

$$\gamma = a \frac{\mu}{10} \quad r_0 \approx \frac{b^2}{8a}$$

$$r_0 \geq a \Rightarrow b \geq 2\sqrt{2}a$$

Characteristics of large
Burgers vectors



The interaction energy between dislocations

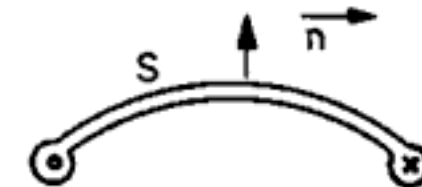
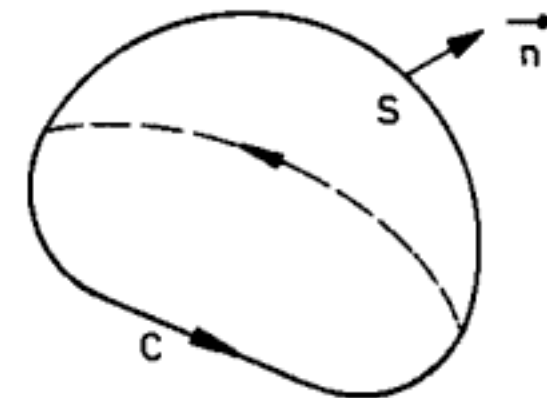
$$E = \frac{1}{2} \int_V \sigma_{ij}^A u_{ij}^A + \frac{1}{2} \int_V \sigma_{ij}^B u_{ij}^B + \frac{1}{2} \int_V \sigma_{ij}^A u_{ij}^B + \frac{1}{2} \int_V \sigma_{ij}^B u_{ij}^A$$

$$\frac{1}{2} \int_V \sigma_{ij}^A u_{ij}^B = \frac{1}{2} \int_V \sigma_{ij}^B u_{ij}^A$$

$$W_I = \int_V \sigma_{ij}^B u_{ij}^A = \int_V \sigma_{ij}^B \frac{\partial u_i^A}{\partial x_j} = \int_V \sigma_{ij}^B \beta_{ji}^A = \int_V \left[\frac{\partial}{\partial x_j} (\sigma_{ij}^B u_i^A) - \frac{\partial \sigma_{ij}^B}{\partial x_j} u_i^A \right] dV$$

= 0

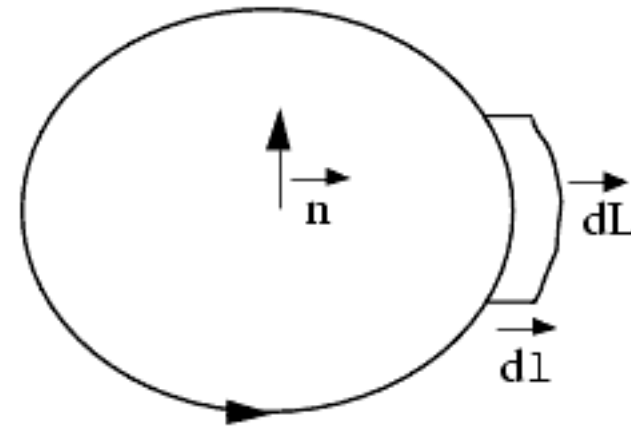
$$W_I = \int_V \frac{\partial}{\partial x_j} (\sigma_{ij}^B u_i^A) dV = \int_S \sigma_{ij}^B u_i^A dS_j$$



$$W_I = \int_S \sigma_{ij}^B u_i^A dS_j = b_i^A \int_S \sigma_{ij}^B dS_j = \vec{b}^A \cdot \int_S \vec{\sigma}^B d\vec{S}$$

Force on a dislocation

$$\vec{F} = -\overrightarrow{\text{grad}} W_I$$



$$dW_I = \vec{b} \left(\overline{\overline{\sigma}} \cdot \overrightarrow{dS} \right) = \left(\vec{b} \cdot \overline{\overline{\sigma}} \right) \overrightarrow{dS} = \left(\vec{b} \cdot \overline{\overline{\sigma}} \right) (\overrightarrow{dl} \wedge \overrightarrow{dL})$$

$$dW_I = - \left(\vec{b} \cdot \overline{\overline{\sigma}} \wedge \overrightarrow{dL} \right) \cdot \overrightarrow{dl} = -d\vec{F} \cdot \overrightarrow{dl}$$

Peach and Koehler force

$$dF_i = -\frac{dW_I}{dl_i} = \left[\left(\vec{b} \cdot \overline{\overline{\sigma}} \right) \wedge \overrightarrow{dL} \right]_i$$

Force on a dislocation

Decomposition of the force acting on the dislocation

a) perpendicular to the slip plane (climb)

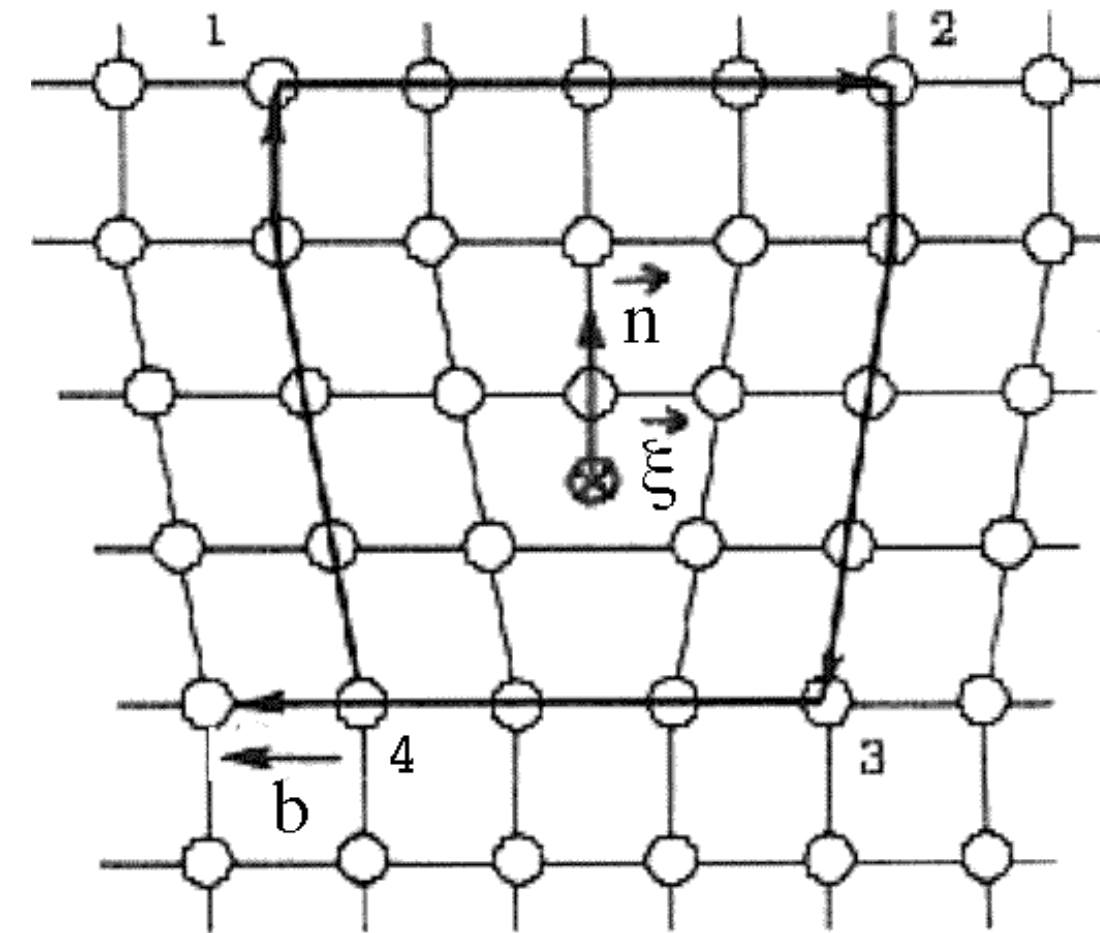
$$F_{\perp} = \left((\vec{b} \cdot \vec{\sigma}) \wedge \vec{\xi} \right) \cdot \vec{n}$$

b) parallel to the dislocation line

$$F_{\parallel} = \left((\vec{b} \cdot \vec{\sigma}) \wedge \vec{\xi} \right) \cdot \vec{\xi} = 0$$

c) in the slip plane

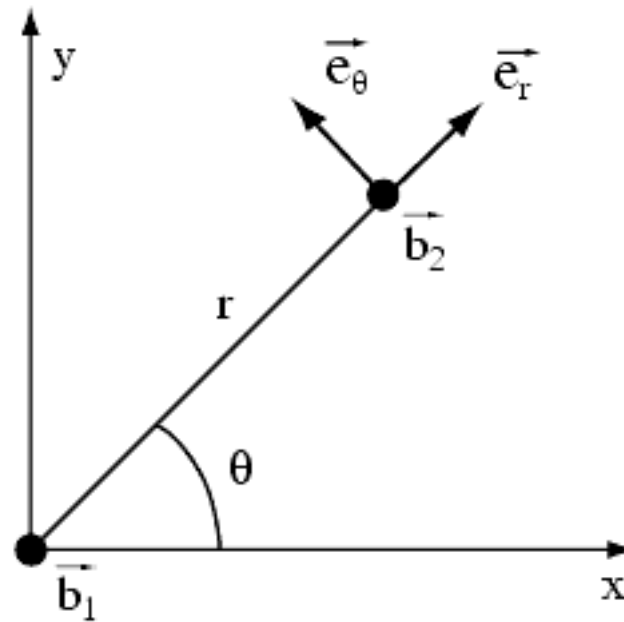
$$F_p = \left((\vec{b} \cdot \vec{\sigma}) \wedge \vec{\xi} \right) \cdot \frac{\vec{b}}{|\vec{b}|} = (\vec{b} \cdot \vec{\sigma}) \cdot \vec{n}$$



$$F_p = \sigma_{ij} b_i n_j$$

Interaction between dislocations

Two parallel screw dislocations



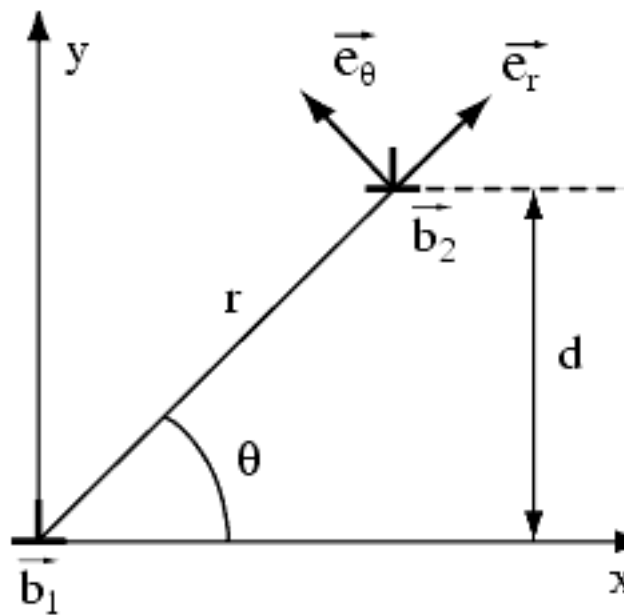
$$\vec{b}_1 = (0, 0, b_1)$$

$$\vec{b}_2 = (0, 0, b_2)$$

$$\sigma_{\theta z} = \frac{\mu b_1}{2\pi r}$$

$$F_r = b_2 \sigma_{\theta z} = \frac{\mu b_1 b_2}{2\pi r} = \pm \frac{\mu b^2}{2\pi r}$$

Two parallel edge dislocations



$$\vec{b}_1 = (b_1, 0, 0)$$

$$\vec{b}_2 = (b_2, 0, 0)$$

$$F_x = b_2 \sigma_{xy}$$

$$F_y = -b_2 \sigma_{xx}$$

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

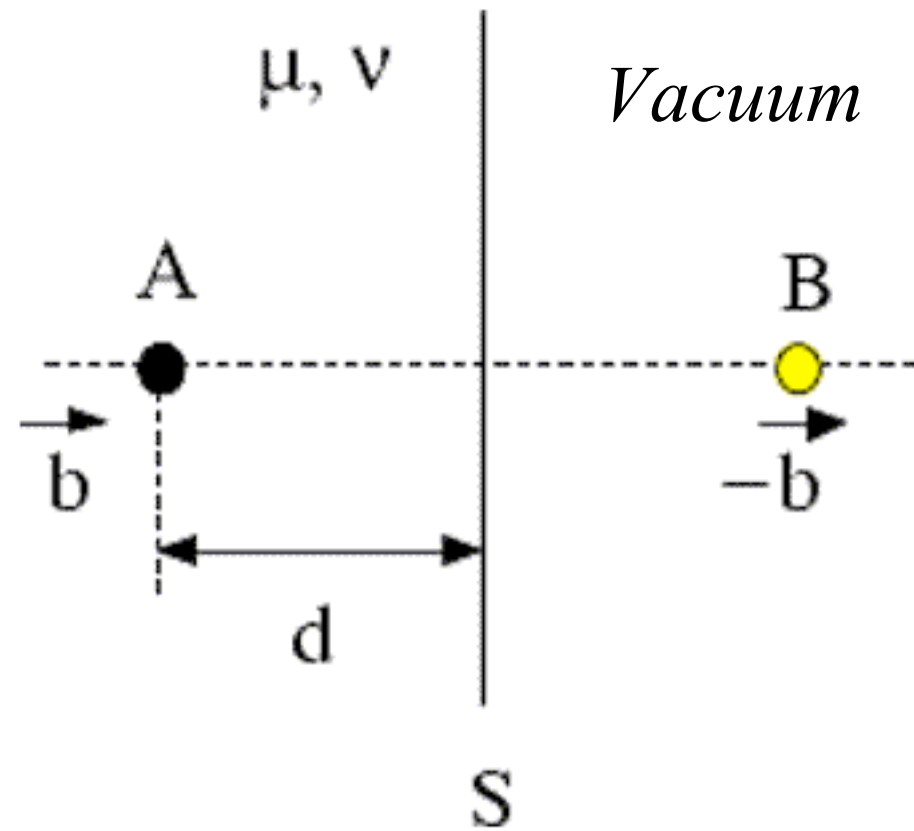
$$\sigma_{xy} = D \frac{\cos \theta \cos 2\theta}{r}$$

$$\sigma_{xx} = -D \frac{\sin \theta (2 + \cos 2\theta)}{r}$$

$$F_x = \frac{\mu b_1 b_2}{2\pi(1-\nu)} \frac{\cos \theta \cos 2\theta}{r}$$

$$F_y = \frac{\mu b_1 b_2}{2\pi(1-\nu)} \frac{\sin \theta (2 + 2 \cos 2\theta)}{r}$$

Surface forces



Self-energy

$$W = \frac{\mu b^2}{4\pi K} \ln \frac{R}{b} \approx \frac{\mu b^2}{4\pi K} \ln \frac{d}{b} \quad K = 1 \text{ or } (1 - \nu)$$

If d decreases, so does the energy:
The surface attracts the dislocation

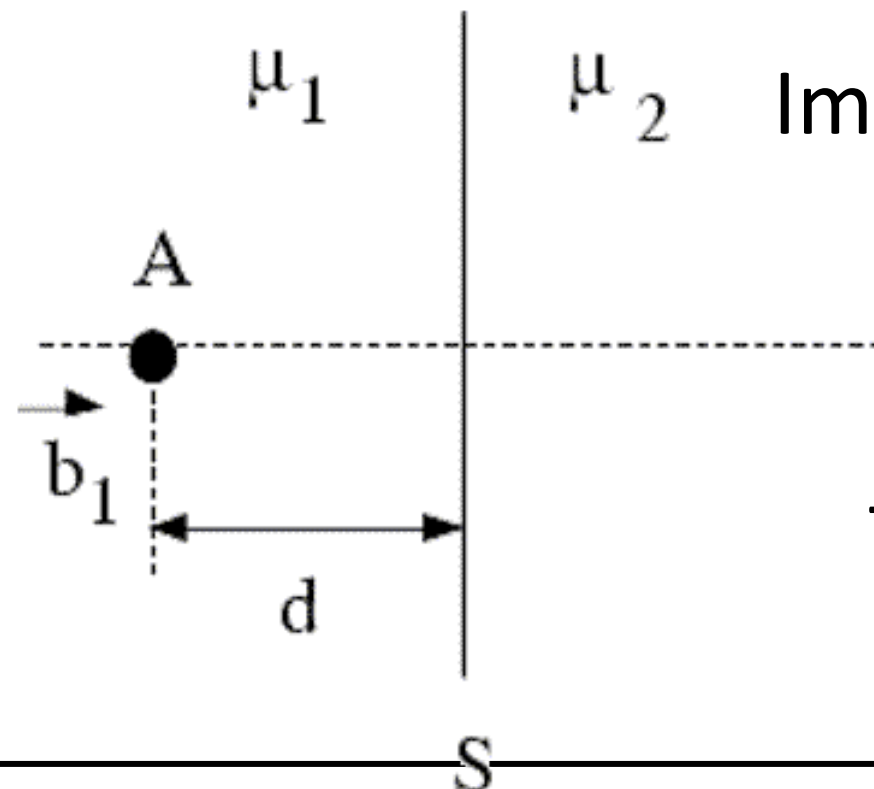
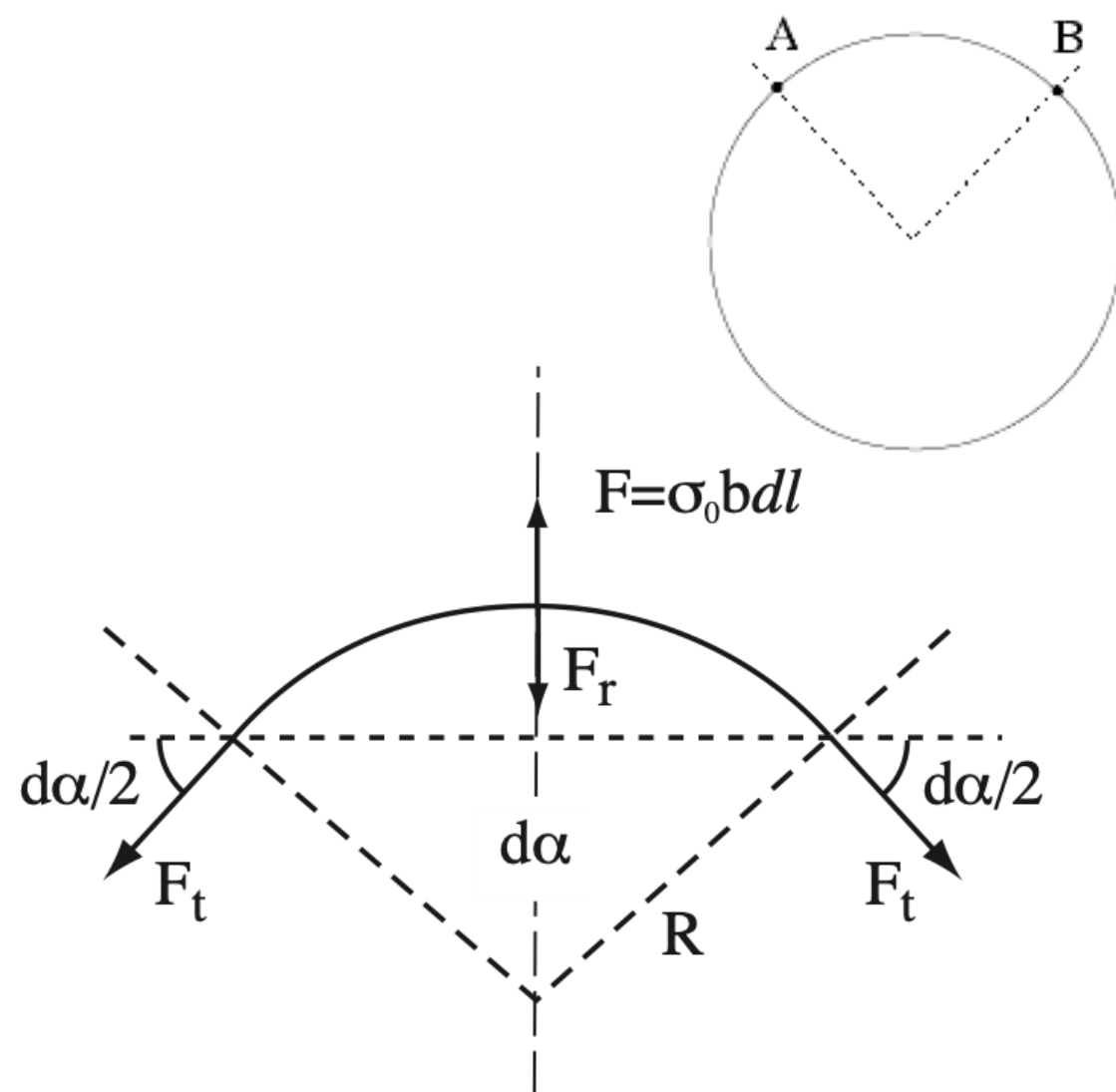


Image force for screw dislocation $F = \frac{\mu b^2}{4\pi d}$

Two environments of different modulus:
the environment with the weaker modulus
attracts the dislocation

Line tension



mixed dislocation which
forms an angle, ψ , with line ξ

$$K = \frac{1-\nu}{1-\nu \cos^2 \psi}$$

$$\tau = \frac{dW}{dl} = \lim_{\delta l \rightarrow 0} \frac{\delta W}{\delta l}$$

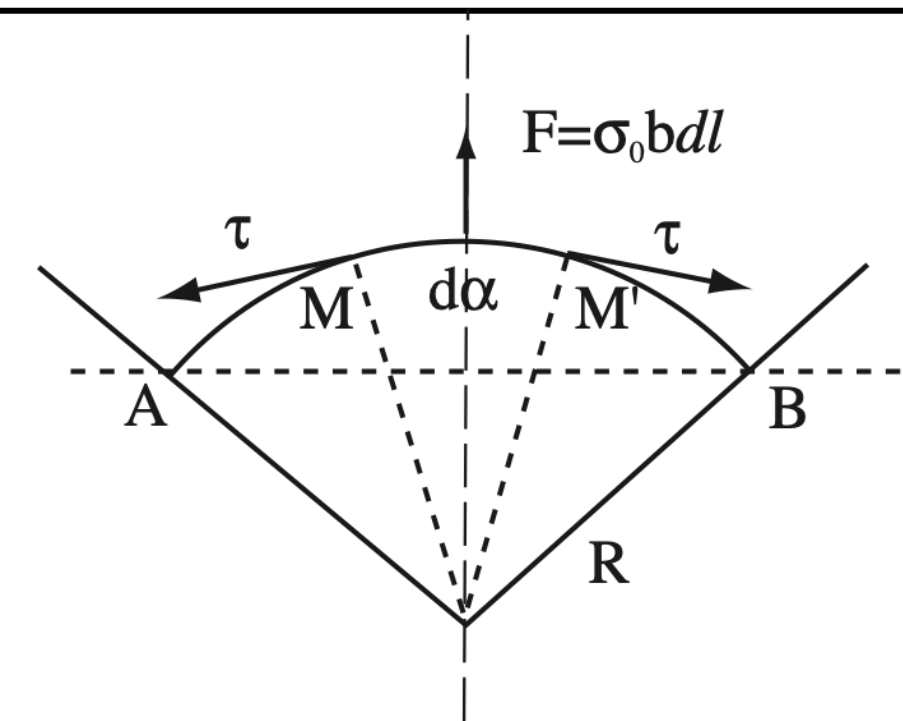
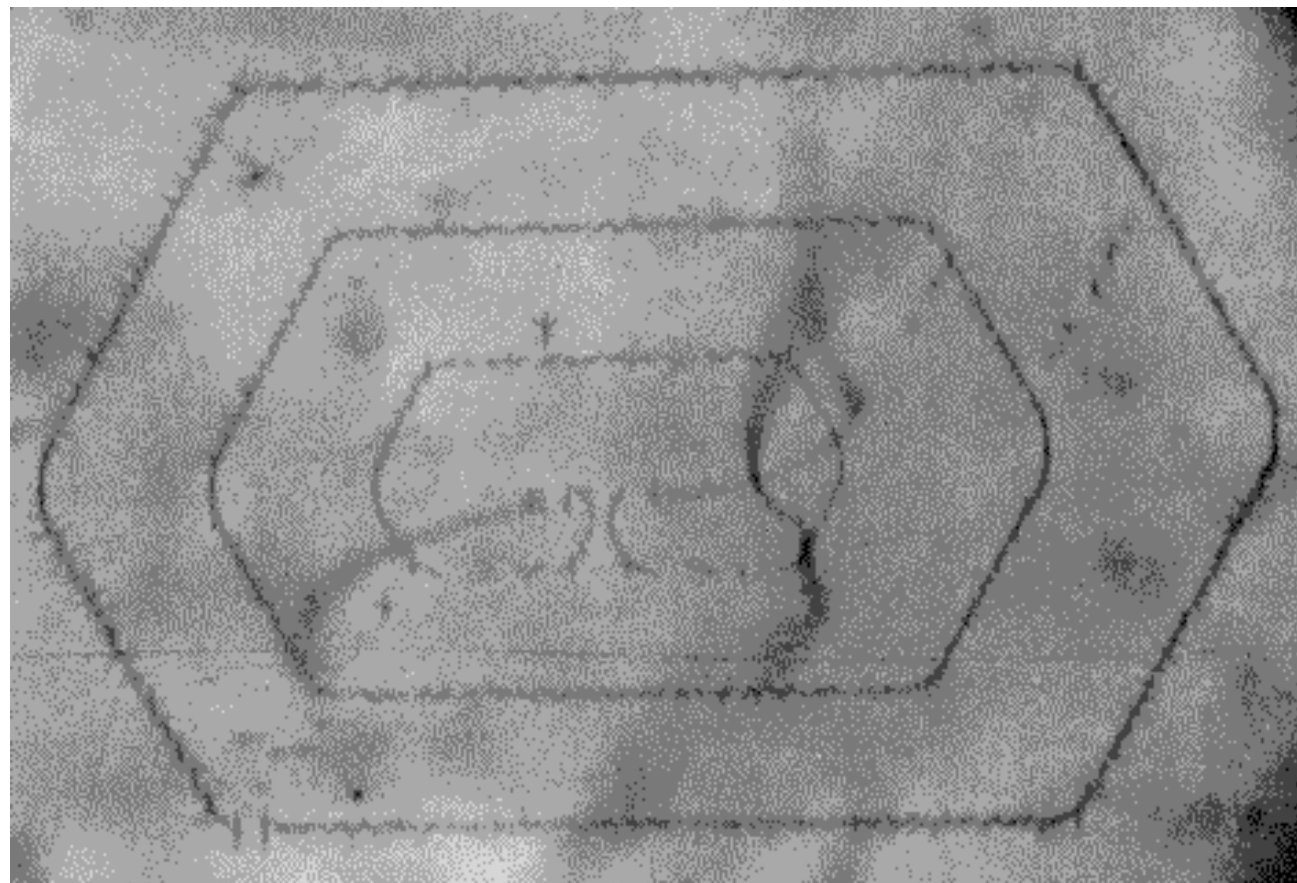
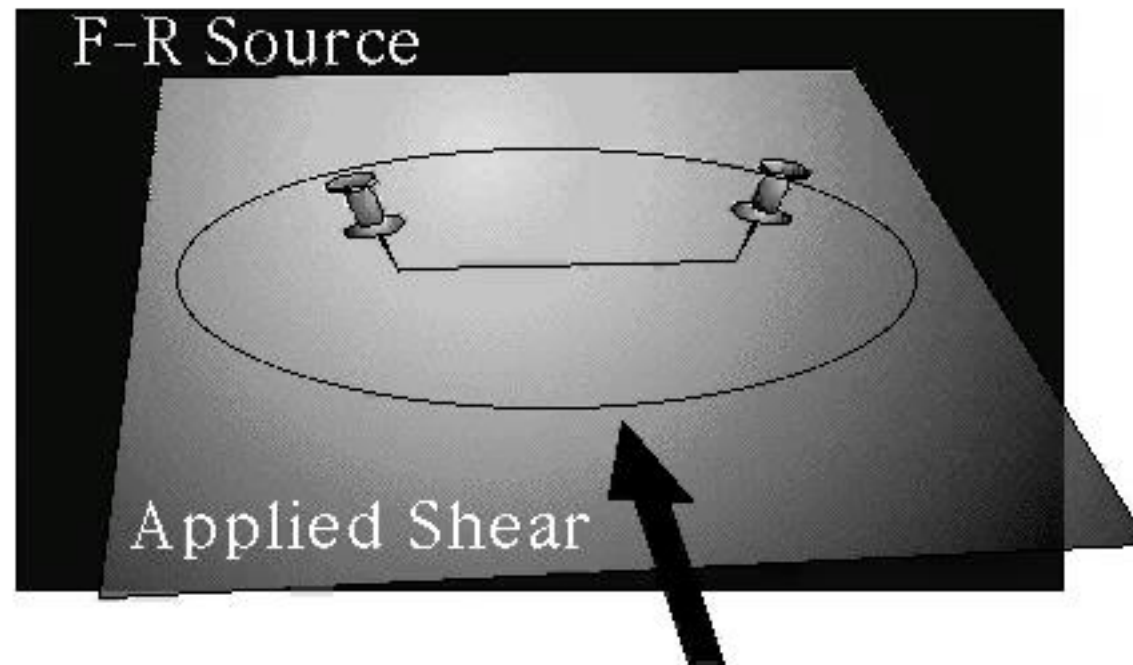
$$F_t = \frac{F_r}{2 \sin(d\alpha / 2)} \approx \frac{F_r}{d\alpha}$$

$$dW = F_t dl \Rightarrow F_t = \frac{dW}{dl}$$

$$W [J / m] = \frac{\mu b^2}{4\pi K} \ln \frac{R}{b} \rightarrow dW [J] = \frac{\mu b^2}{4\pi K} \ln \frac{R}{b} dl$$

$$\tau [N] = \frac{\mu b^2}{4\pi K} \ln \frac{R}{b} \approx \mu b^2$$

Application of the line tension: Frank Read source



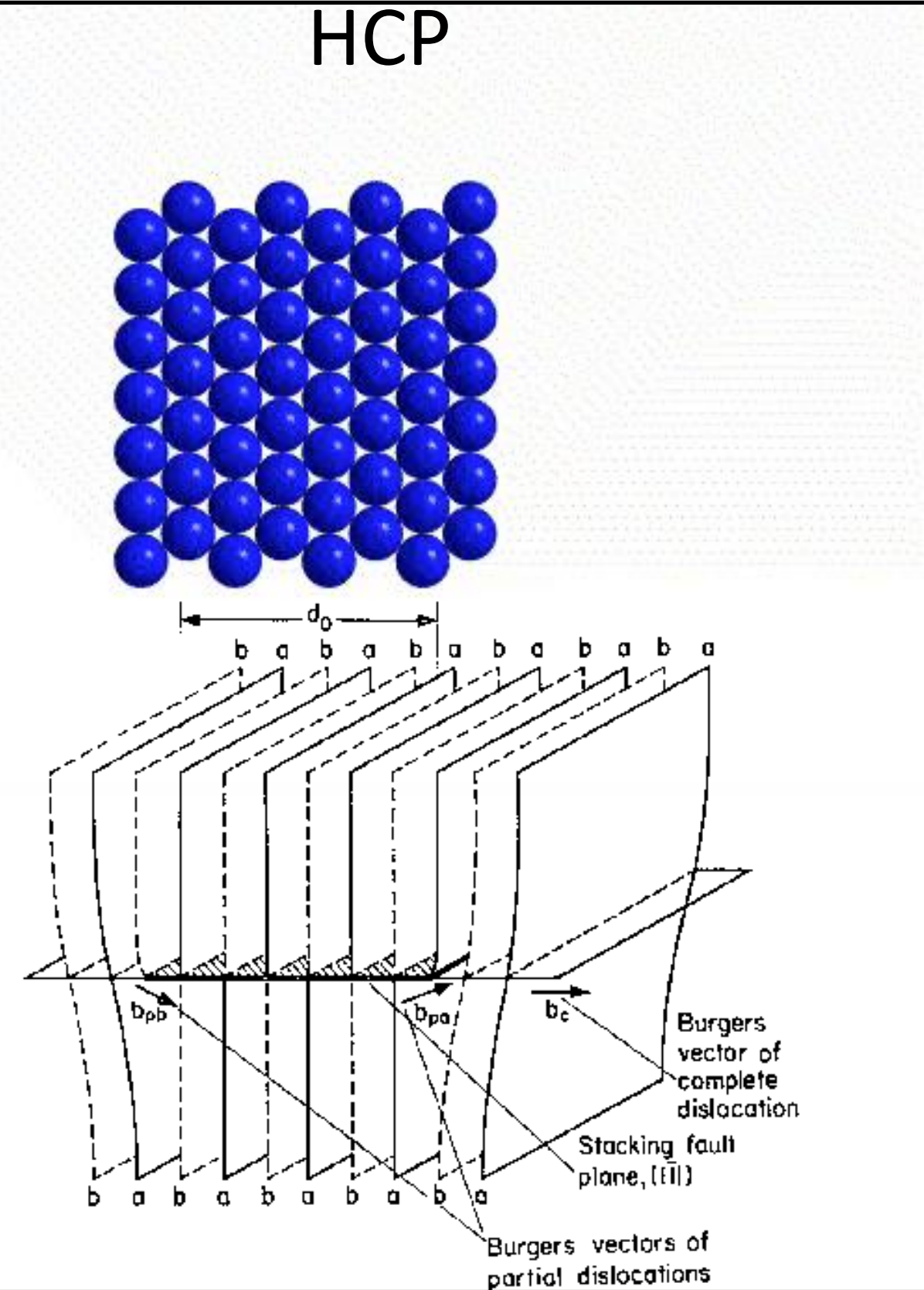
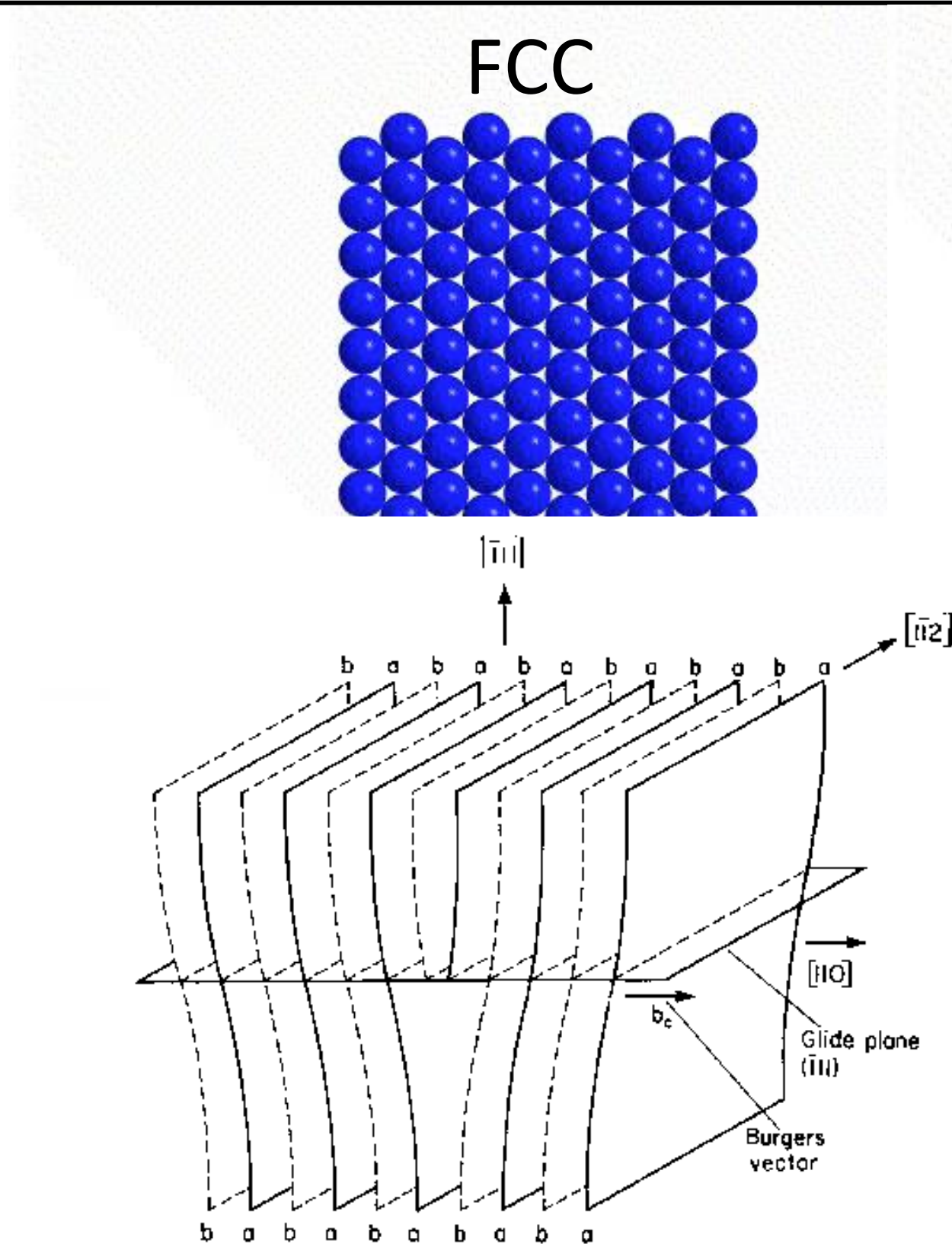
$$2\tau \sin(d\alpha / 2) = \sigma_0 bdl = \sigma_0 bRd\alpha$$

$$R = \frac{\tau}{\sigma_0 b} \geq \frac{l}{2} \Rightarrow \sigma_0 \leq \frac{2\tau}{bl}$$

$$\sigma_0 = \frac{2\tau}{bl} \approx \frac{\mu b}{l} \sim 2.5 \cdot 10^{-5} \mu$$

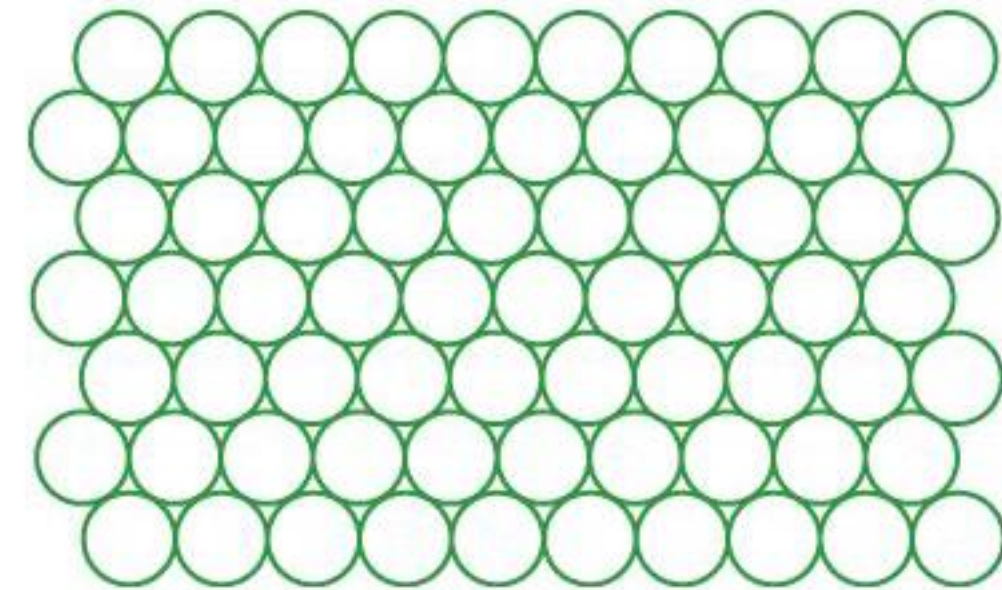
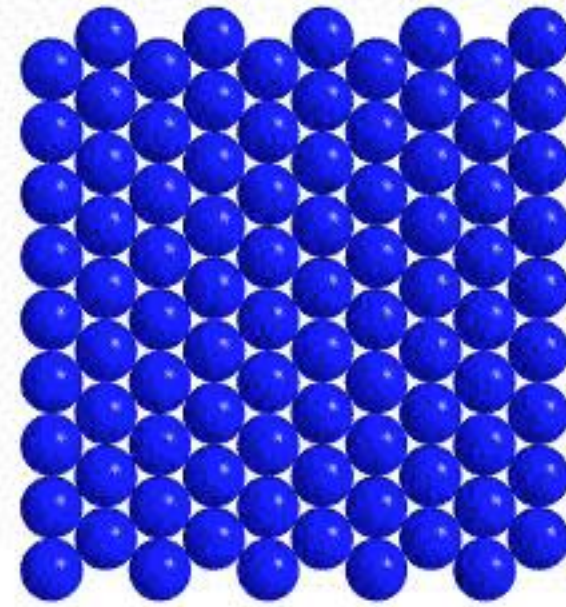
$$\sigma_0 \sim 2.4 \text{ MPa for copper}$$

Dislocations in face-centered cubic metals

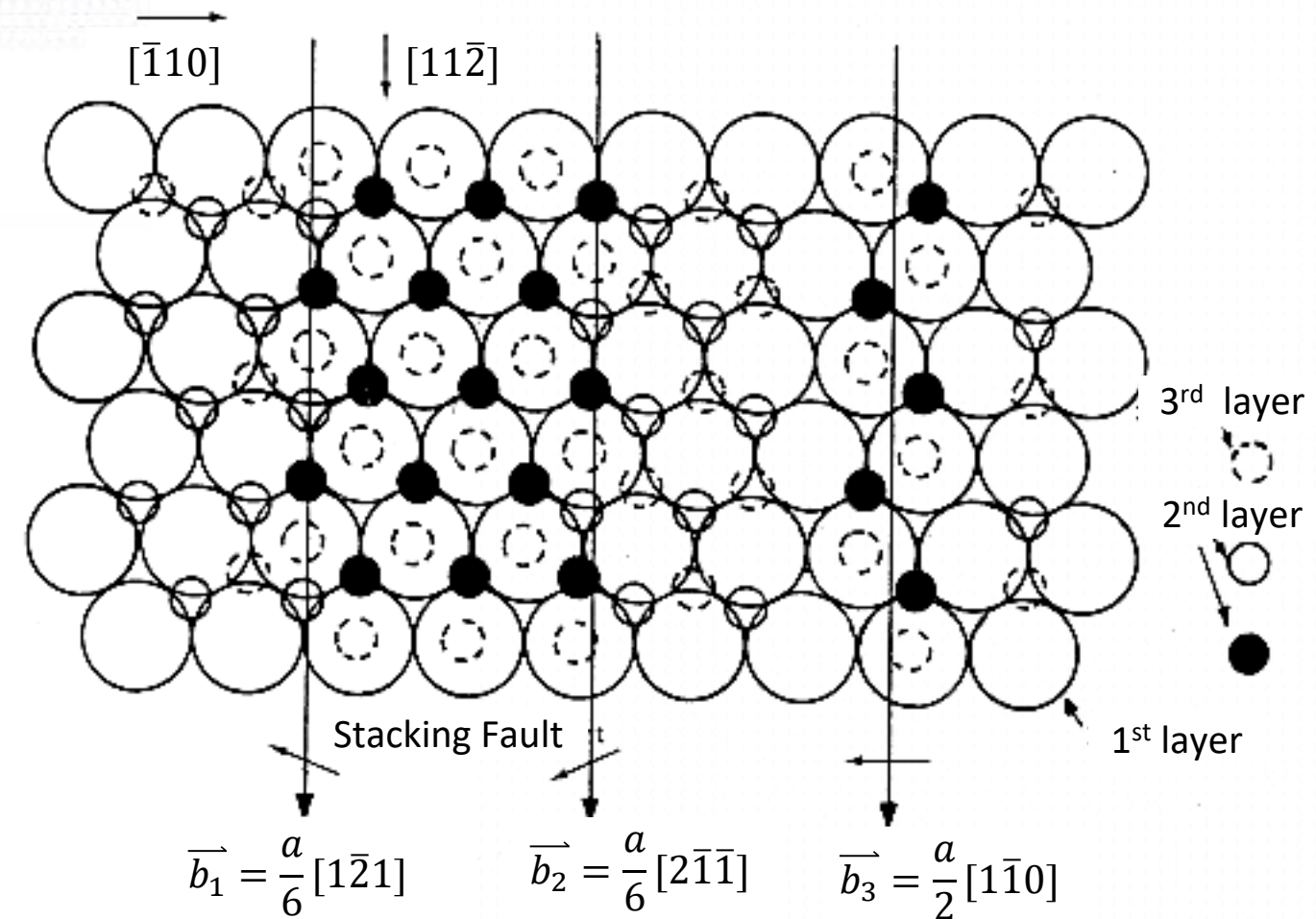
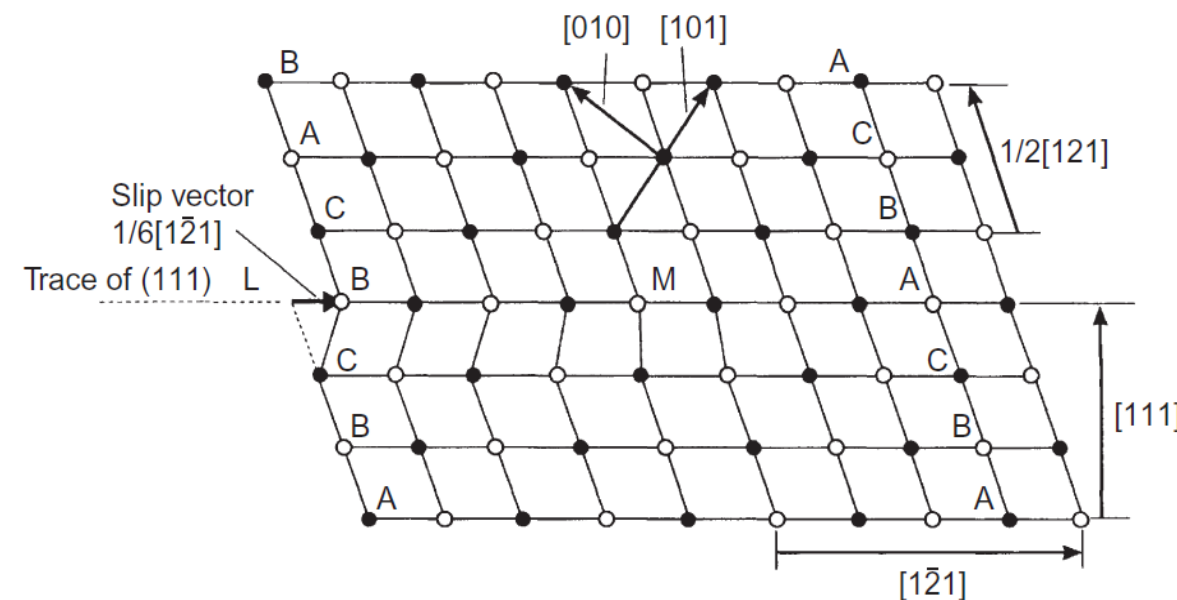


Dislocations in face-centered cubic metals

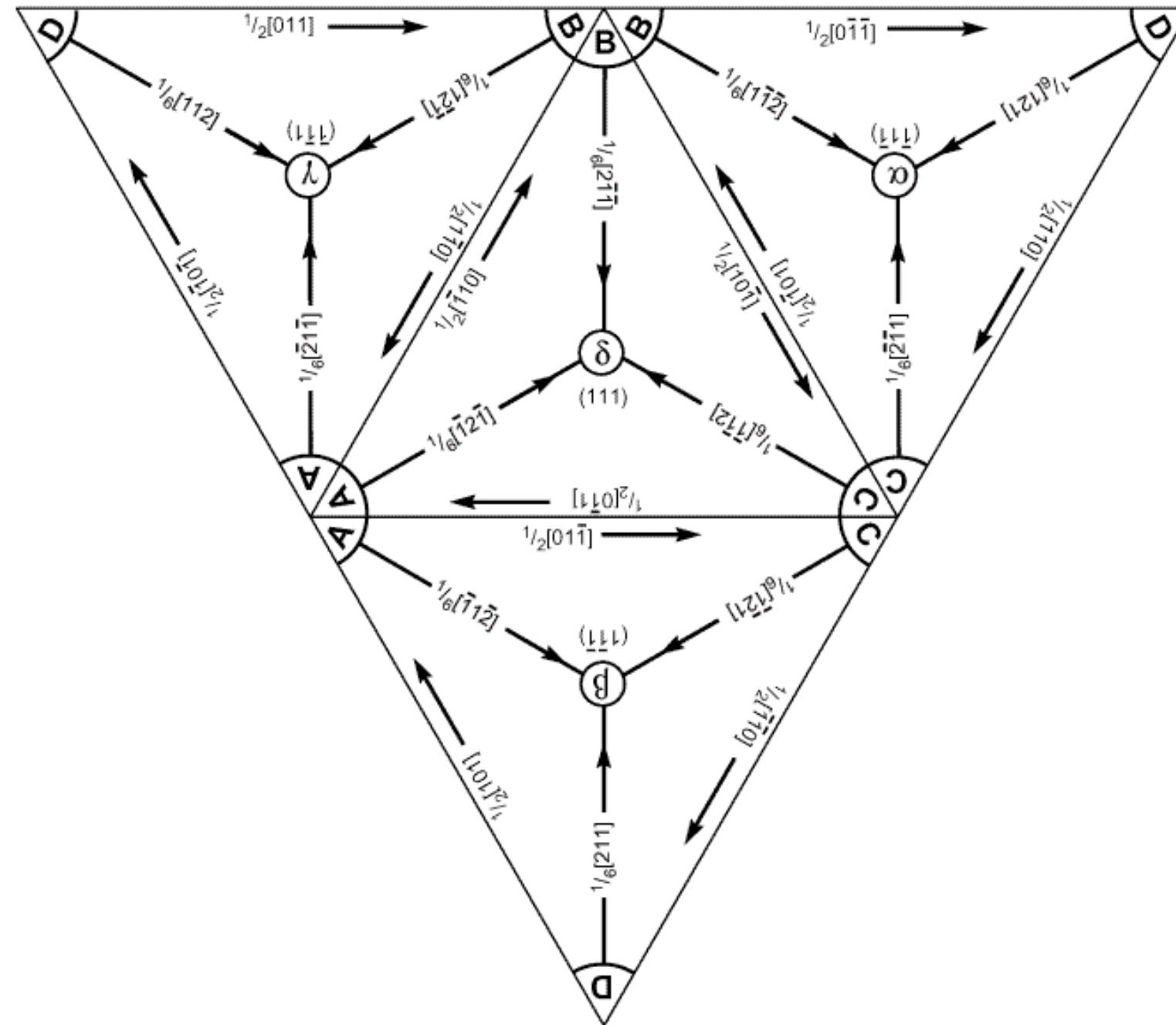
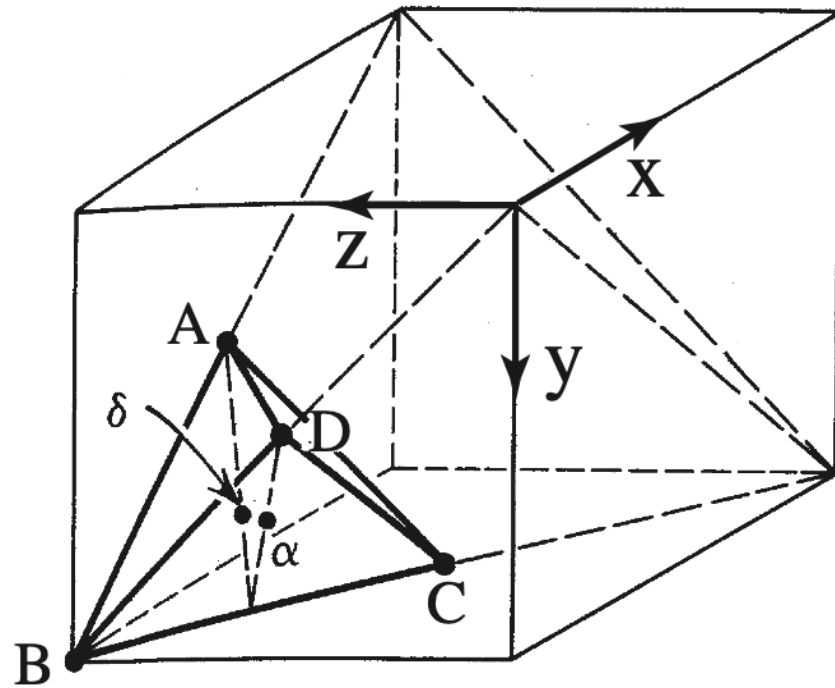
FCC



Shockley partial



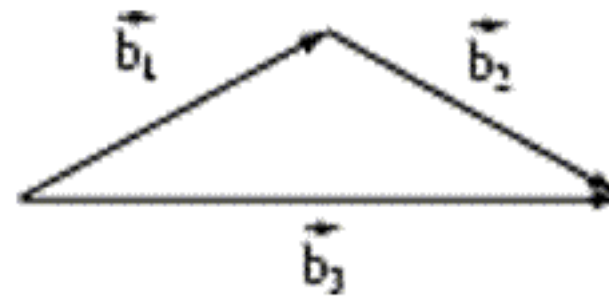
Thompson tetrahedron



Energy calculation

$$W = \frac{\mu b^2}{4\pi K} \ln \frac{R}{b} \approx \mu b^2$$

$$\frac{a}{2}[1\bar{1}0] = \frac{a}{6}[2\bar{1}\bar{1}] + \frac{a}{6}[1\bar{2}1]$$



$$\vec{b}_3 = \vec{b}_1 + \vec{b}_2$$

Frank's Rule

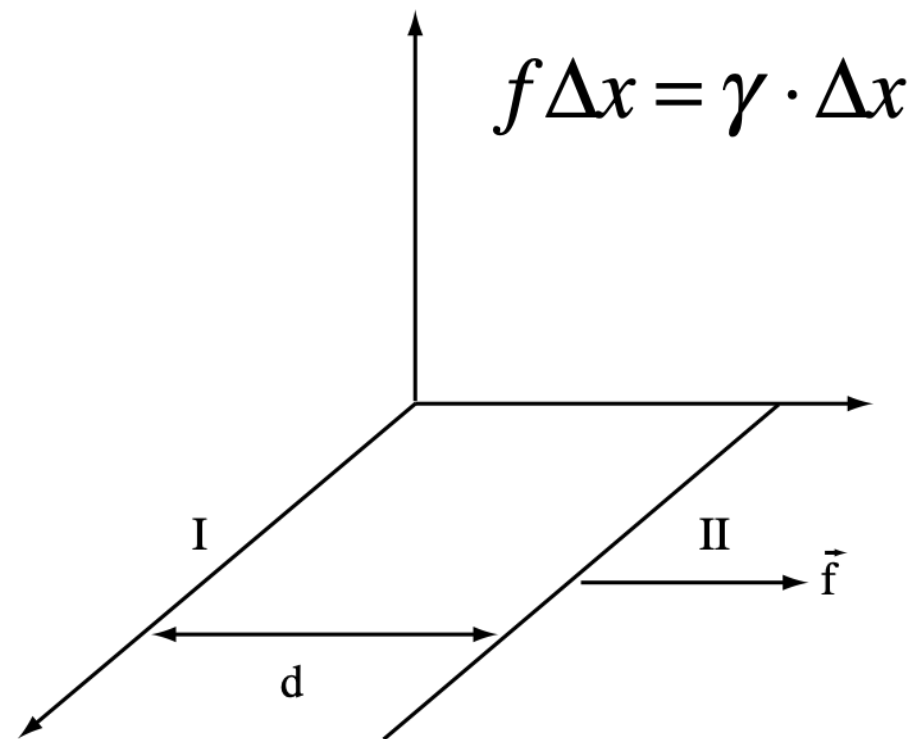
$$b_1^2 + b_2^2 < b_3^2$$

Dislocation dissociates
into partials

$$b_1^2 + b_2^2 > b_3^2$$

Dislocation does not
dissociate into partials

Energy of stacking fault



applications

Copper: $\mu = 4.85 \times 10^4 \text{ J cm}^{-3}$ $\gamma = 4 \text{ } \mu\text{J cm}^{-2}$

$a = 3.62 \times 10^{-8} \text{ cm}$ $\nu = 0.33$ $d = 3.7 \text{ nm}$

Aluminum: $\mu = 2.8 \times 10^4 \text{ J cm}^{-3}$ $\gamma = 20 \text{ } \mu\text{J cm}^{-2}$

$a = 4.05 \times 10^{-8} \text{ cm}$ $\nu = 0.33$ $d = 0.54 \text{ nm}$

γ is the stacking fault energy
we show (exercise) that

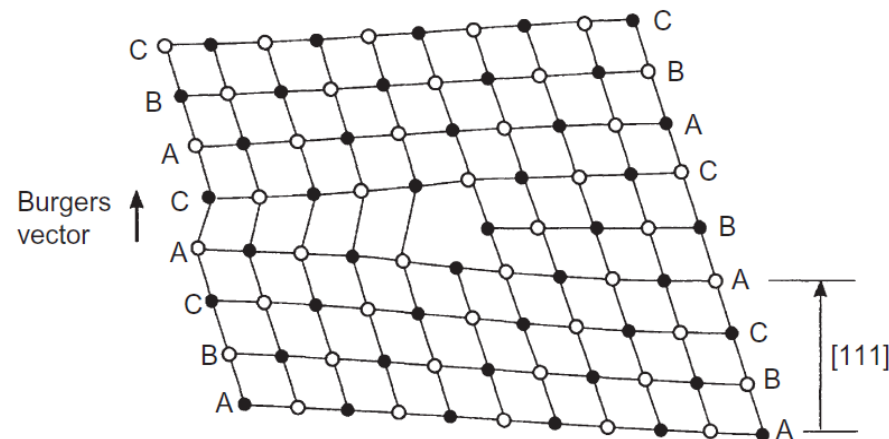
$$f_y = \frac{\mu}{2\pi d} \left(\frac{b_e^I b_e^{II}}{1-\nu} + b_s^I b_s^{II} \right)$$

$$b_y = b_e^{II} = \frac{a}{2\sqrt{2}} \quad b_x = b_s^{II} = -b_s^I = -\frac{a}{2\sqrt{6}}$$

$$\frac{\mu}{2\pi d} \left(\frac{b_e^2}{1-\nu} \right) = \gamma + \frac{\mu b_s^2}{2\pi d} \Rightarrow d = \frac{(2+\nu)\mu a^2}{48\pi(1-\nu)\gamma}$$

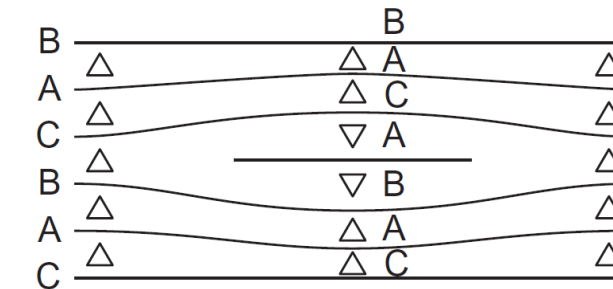
Sessile dislocations

Frank partial dislocation

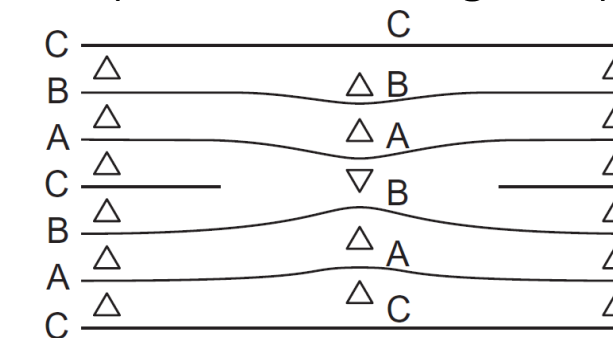


$$\vec{b} = \overrightarrow{A\alpha} = \frac{a}{3}[\bar{1}1\bar{1}]$$

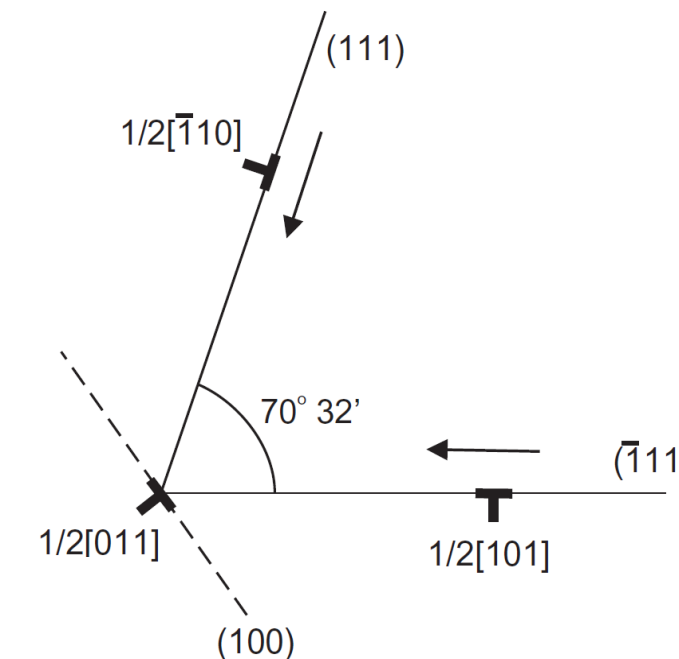
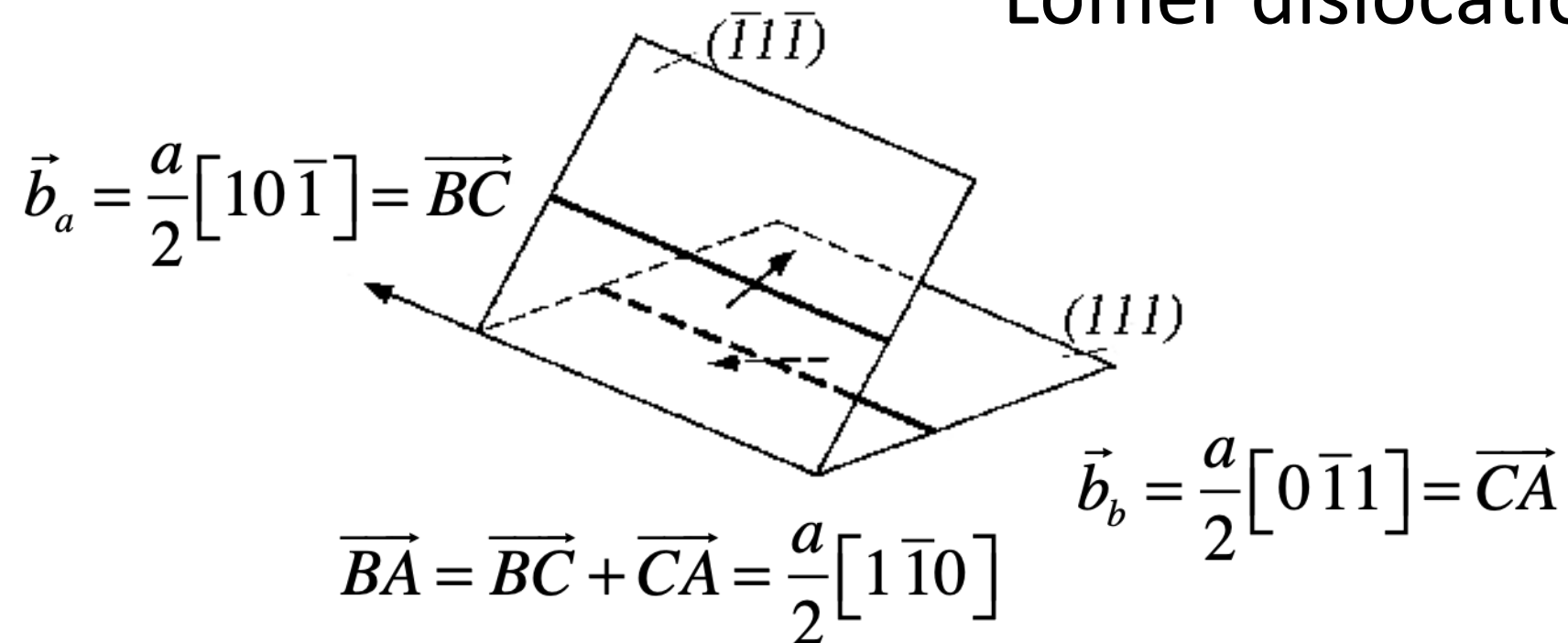
Positive Frank dislocation (extrinsic stacking fault)



Negative Frank dislocation (intrinsic stacking fault)



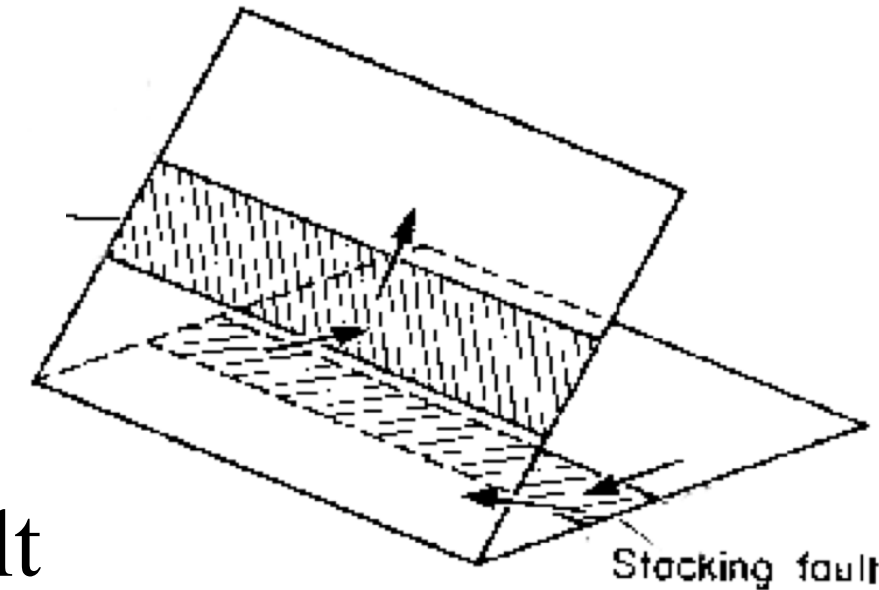
Lomer dislocation



Sessile dislocations

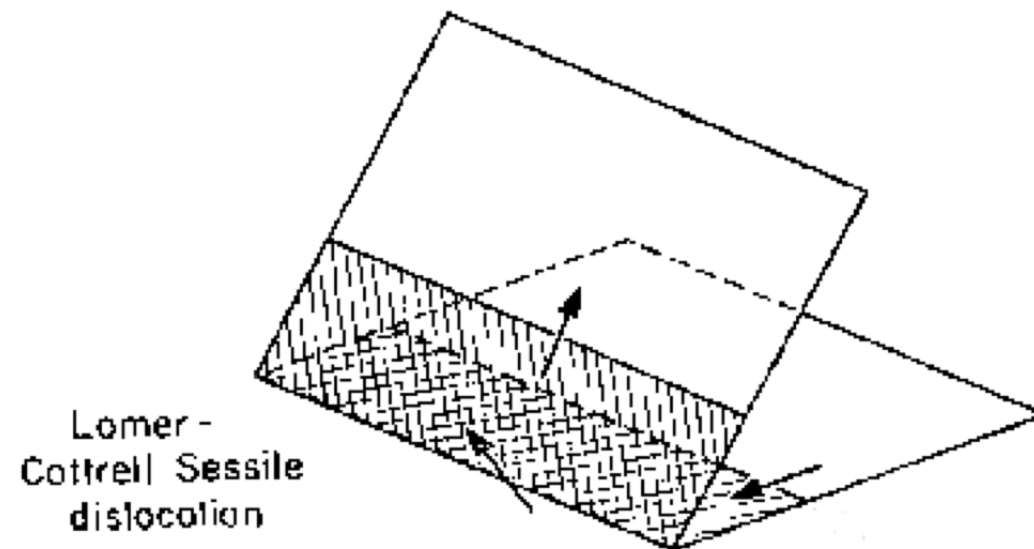
Lomer Cottrell dislocation

$$\overrightarrow{CA} = \overrightarrow{C\beta} + \overrightarrow{\beta A} = \frac{a}{6}[\bar{1}\bar{2}1] + \frac{a}{6}[1\bar{1}2] = \frac{a}{2}[0\bar{1}1]$$



Stacking fault

$$\overrightarrow{BC} = \overrightarrow{B\alpha} + \overrightarrow{\alpha C} = \frac{a}{6}[1\bar{1}2] + \frac{a}{6}[21\bar{1}] = \frac{a}{2}[10\bar{1}]$$

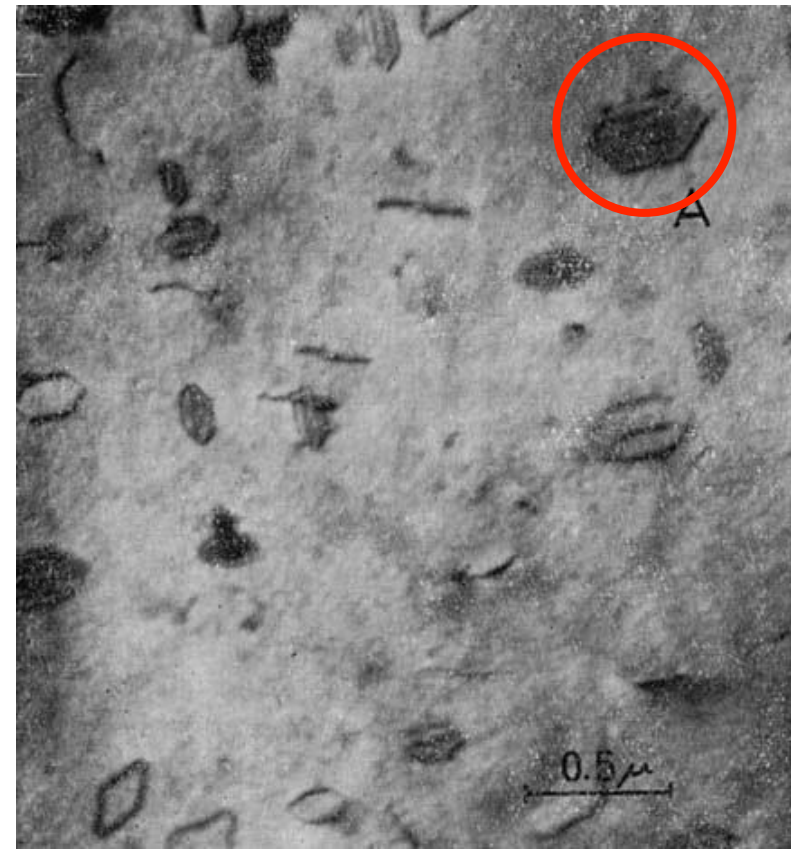


$$\overrightarrow{\alpha\beta} = \overrightarrow{\alpha C} + \overrightarrow{C\beta} = \frac{a}{6}[21\bar{1}] + \frac{a}{6}[\bar{1}\bar{2}1] = \frac{a}{6}[1\bar{1}0]$$

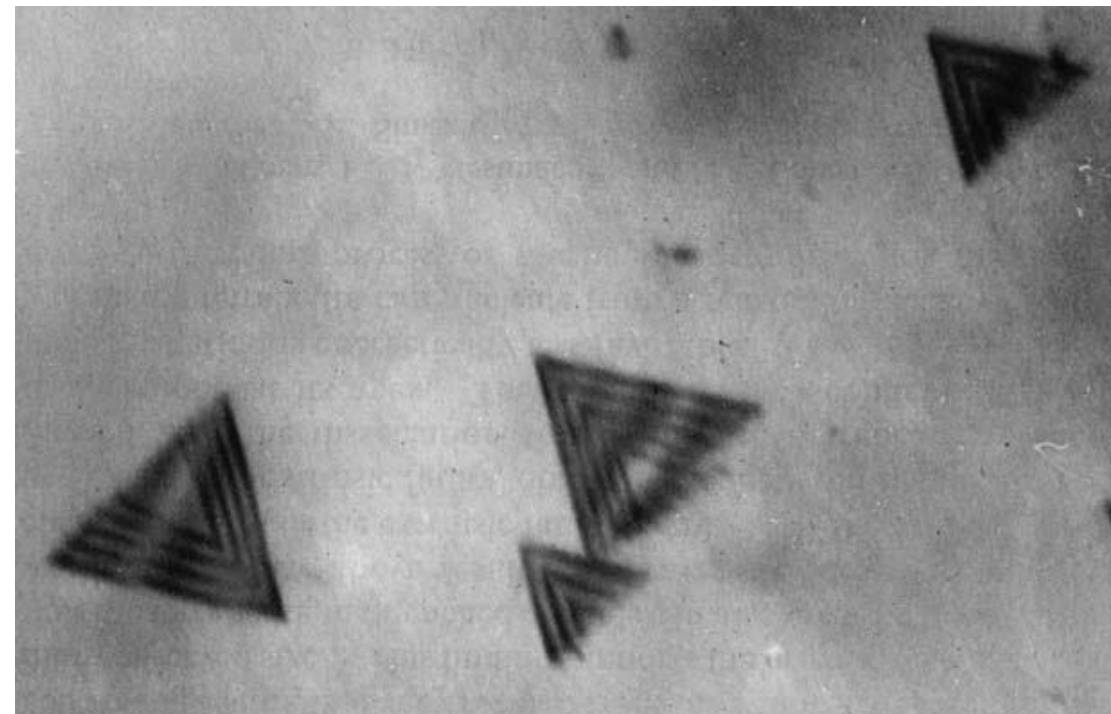
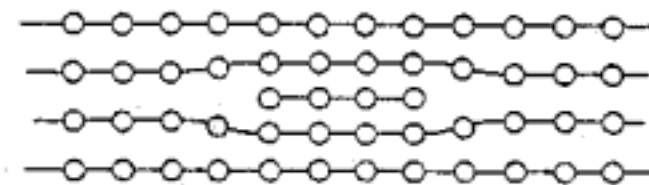
$$\frac{a^2}{6} + \frac{a^2}{6} > \frac{a^2}{18}$$

$$\frac{1}{6}[21\bar{1}] + \frac{1}{6}[\bar{1}\bar{2}1] + \frac{1}{6}[1\bar{1}0] = \frac{1}{2}[1\bar{1}0] \rightarrow \frac{a^2}{6} + \frac{a^2}{6} + \frac{a^2}{18} < \frac{a^2}{2}$$

Prismatic loops

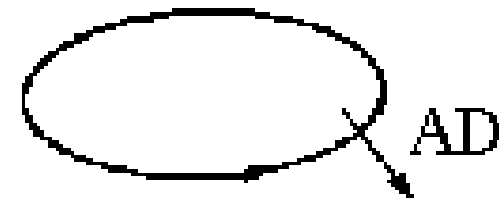
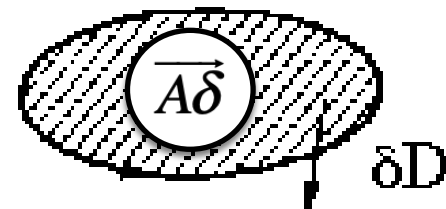
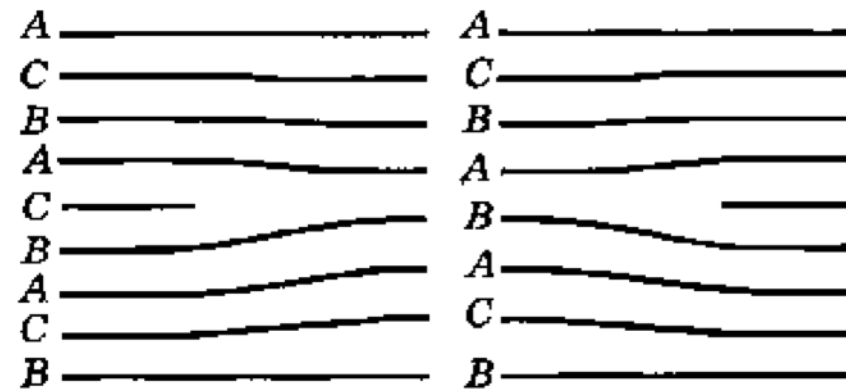


Al



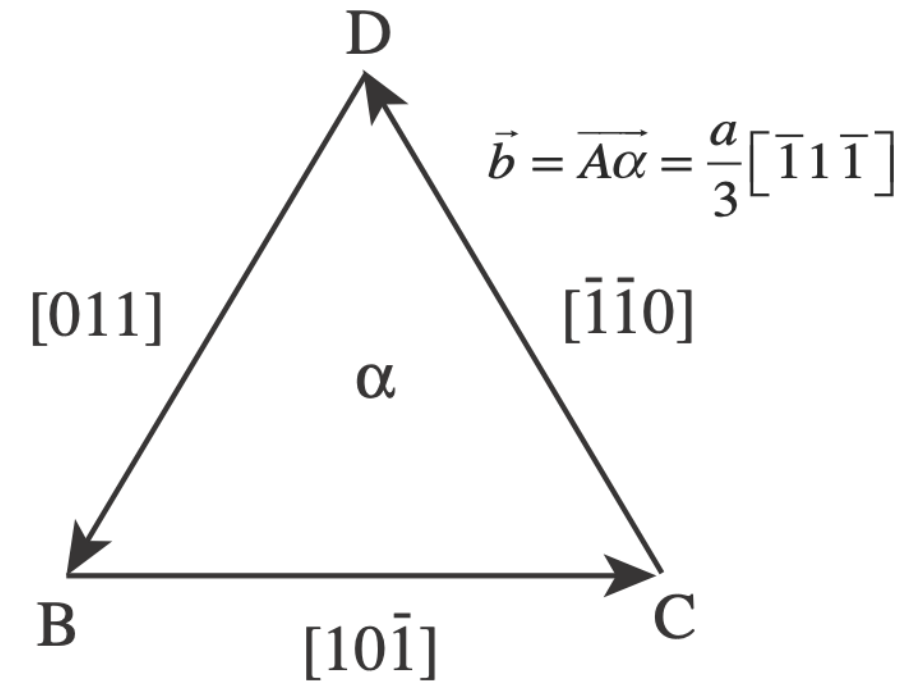
Au

Prismatic loops



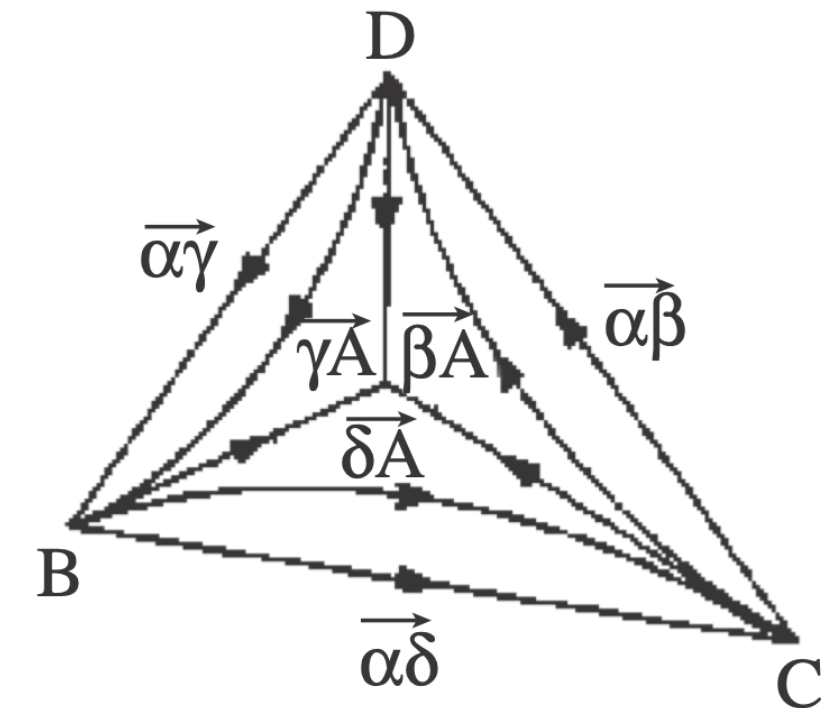
$$\overrightarrow{A\delta} + \overrightarrow{\delta D} = \overrightarrow{AD} = \frac{a}{2}[\bar{1}0\bar{1}]$$

Al: high fault energy



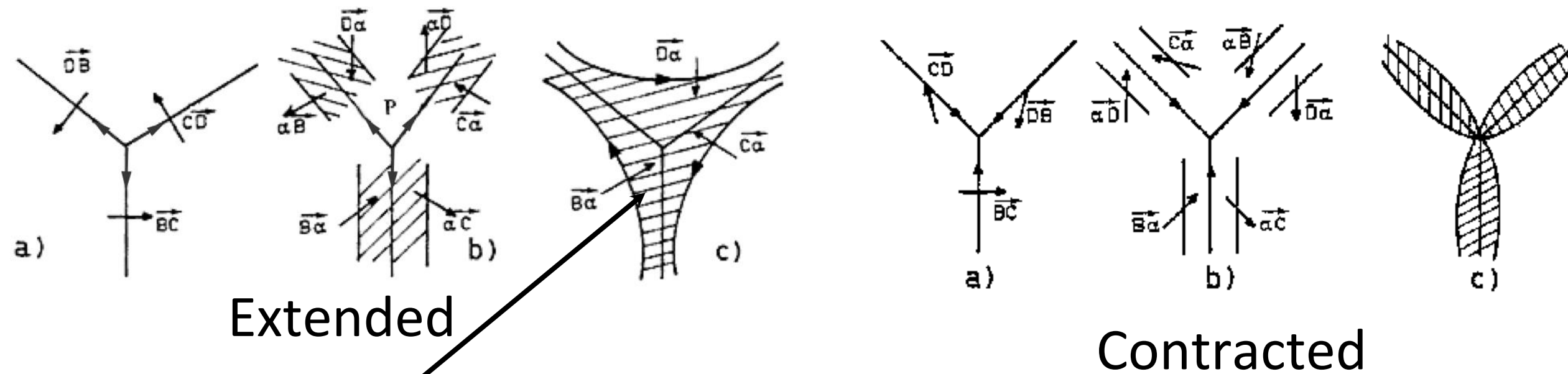
$$\frac{1}{3}[\bar{1}1\bar{1}] = \frac{1}{6}[\bar{1}2\bar{1}] + \frac{1}{6}[\bar{1}0\bar{1}]$$

$$\frac{a^2}{3} > \frac{a^2}{6} + \frac{a^2}{18}$$



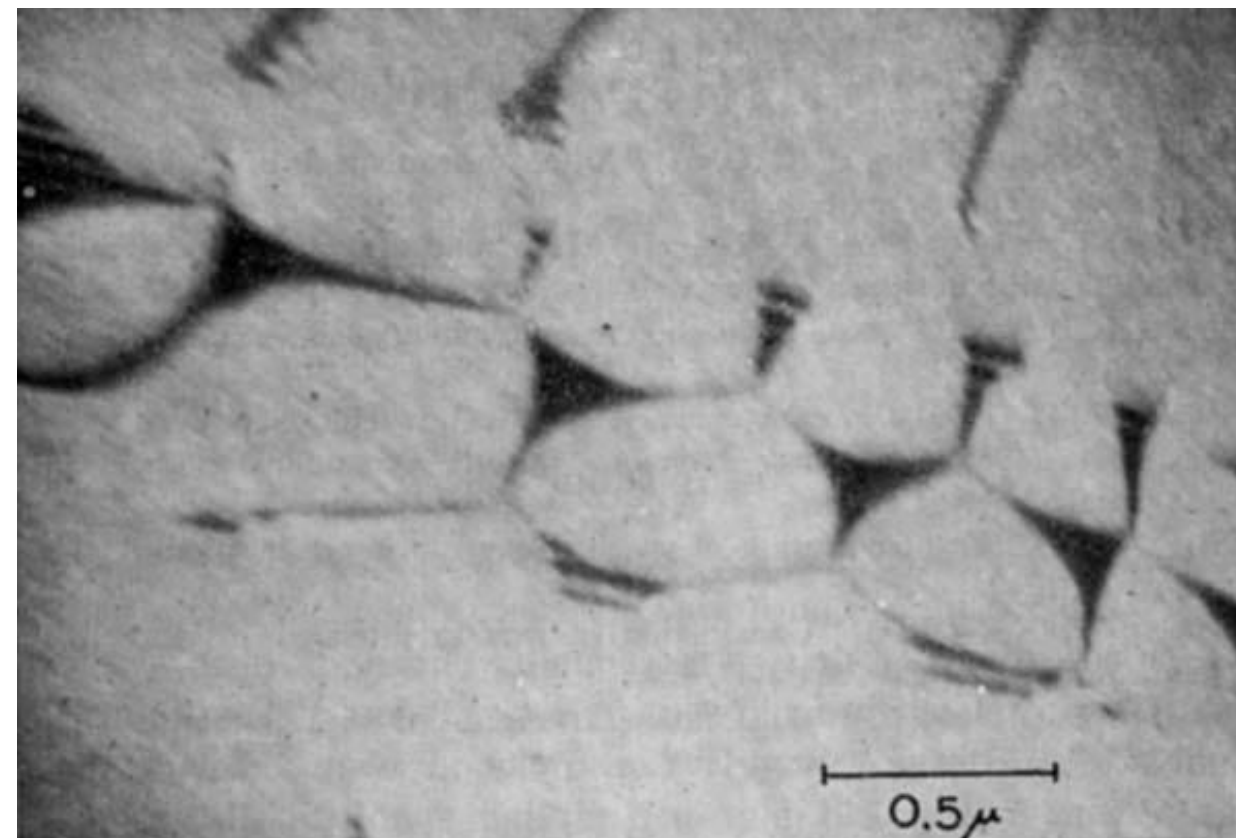
Au: low fault energy

Dislocation nodes in FCC metals

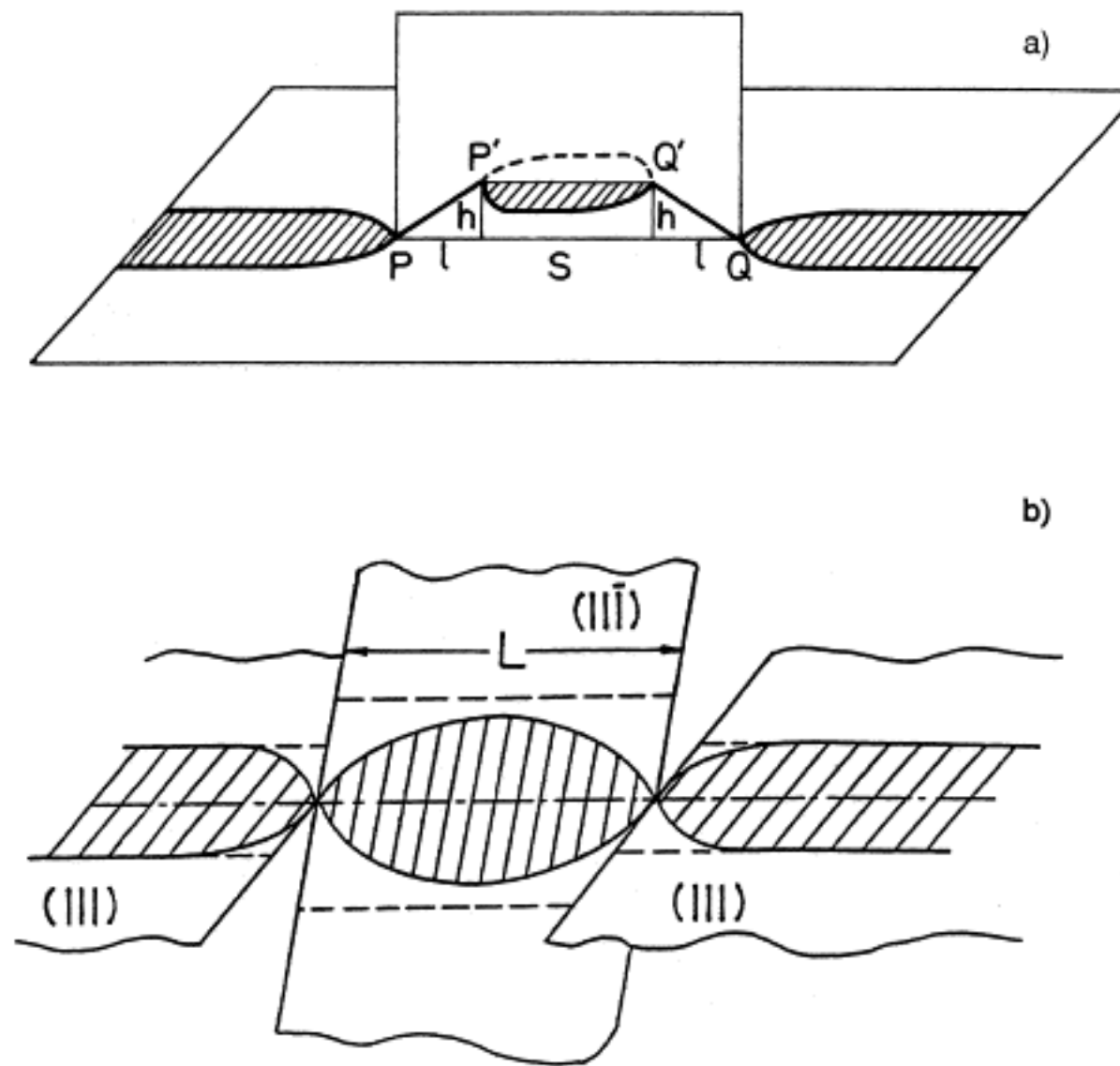


$$\gamma = \frac{\tau}{R}$$

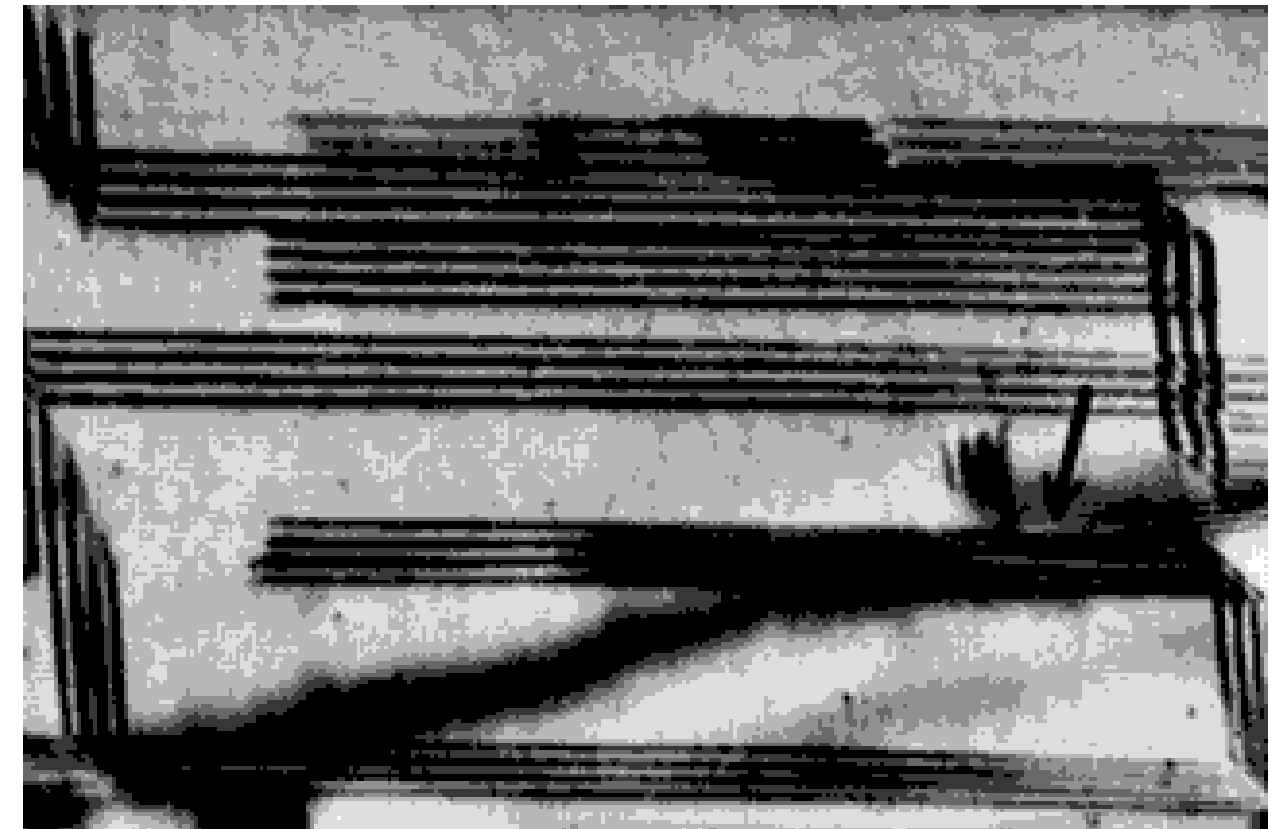
$$\gamma = \frac{\alpha \mu b_s^2}{R}$$



Cross slip in FCC metals



Stair-Rod Dislocations



Cu-10%Fe