Physics of Materials

Chapter 7: Elasticity Theory of Dislocations

Dr. Thomas LaGrange

Masters Course PHYS-307

Fall 2025

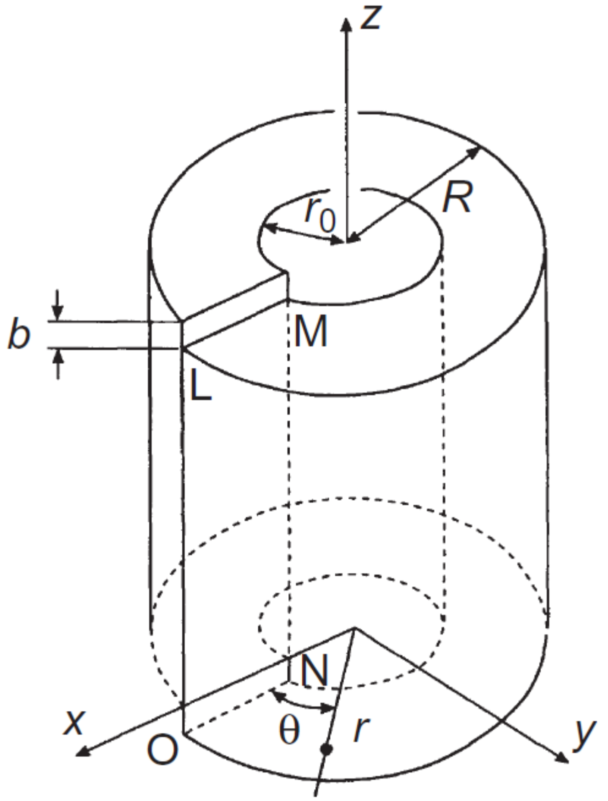
Stress field around a (screw) dislocation

1) Equilibrium (Naiver-Stokes) equation

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

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

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

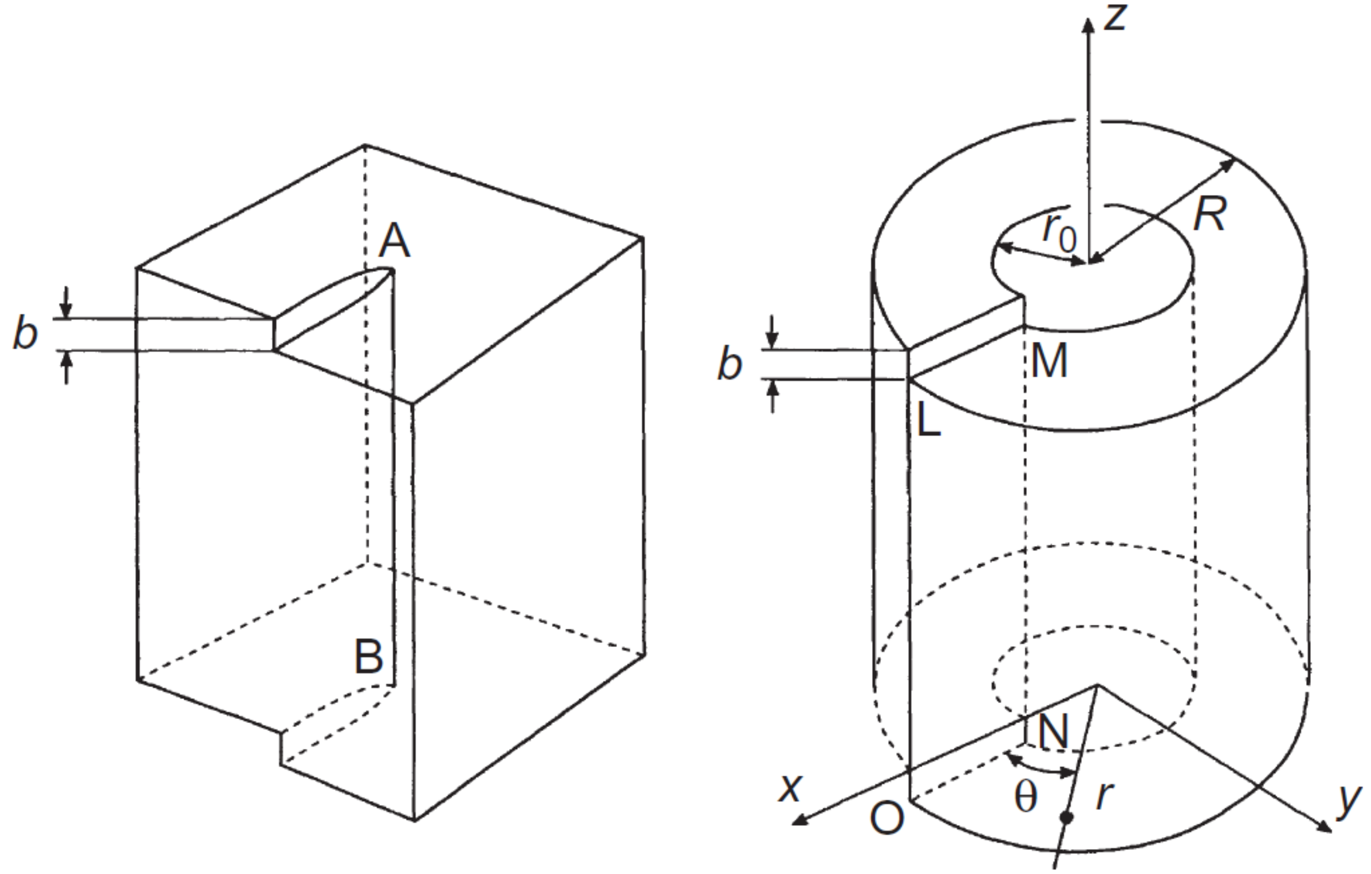
$$u_r=u_\theta=0 \qquad u_z=\frac{b\theta}{2\pi}$$

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

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

thomas.lagrange@epfl.ch • www.epfl.ch• lumes.epfl.ch• moodle.epfl.ch• PHYS-307

Stress field around a (screw) dislocation



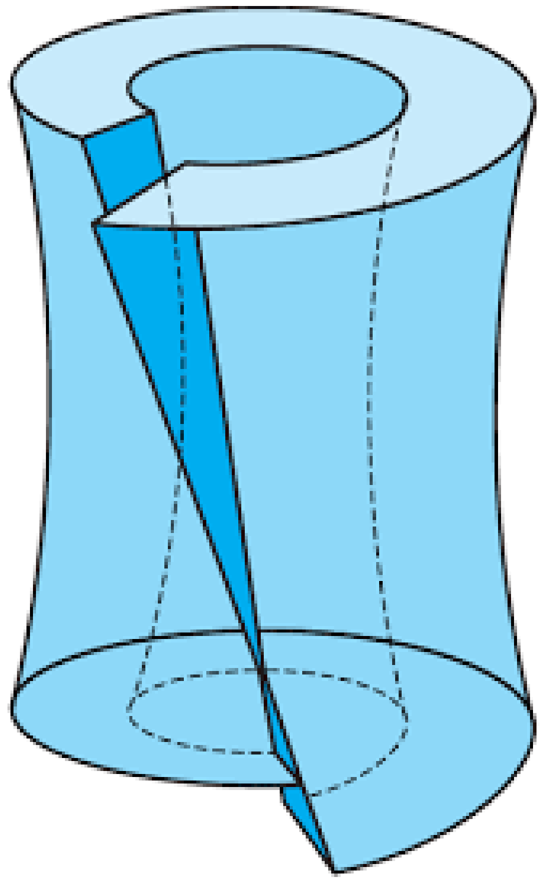
In cartesian coordinates

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

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

thomas.lagrange@epfl.ch • www.epfl.ch• lumes.epfl.ch• moodle.epfl.ch• PHYS-307

Screw dislocation (finite length)



The previous solution is valid for an infinite medium: non-zero stress at the surface

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

We suppose the presence of a counter-torque

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

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

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

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

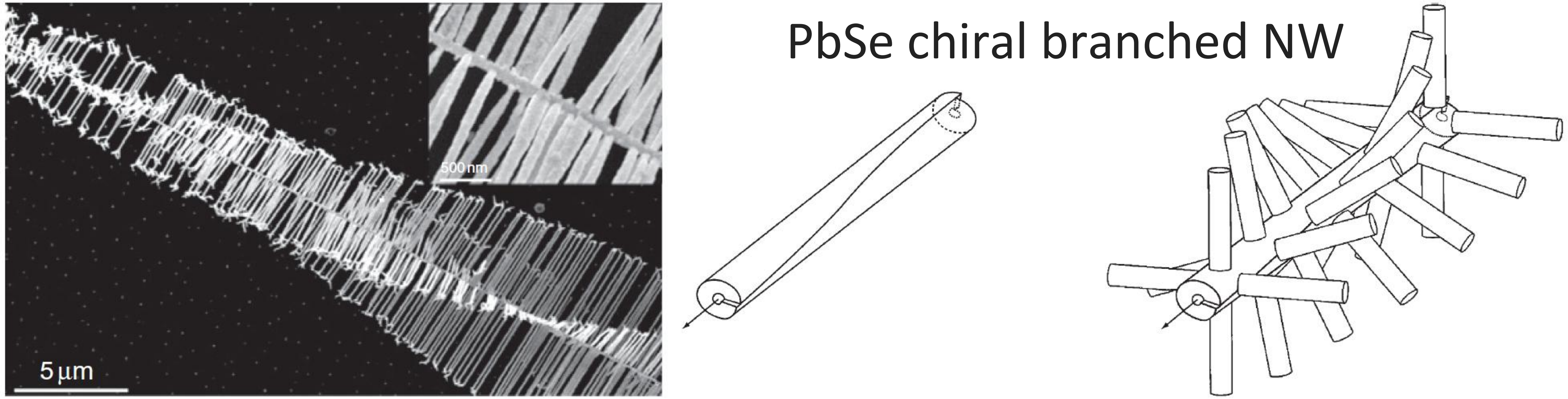
$$M'_z = -M_z \rightarrow A = \frac{b}{\pi}\frac{R^2 - r_0^2}{R^4 - r_0^4}$$

solution

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

Screw dislocation and Eshelby twist

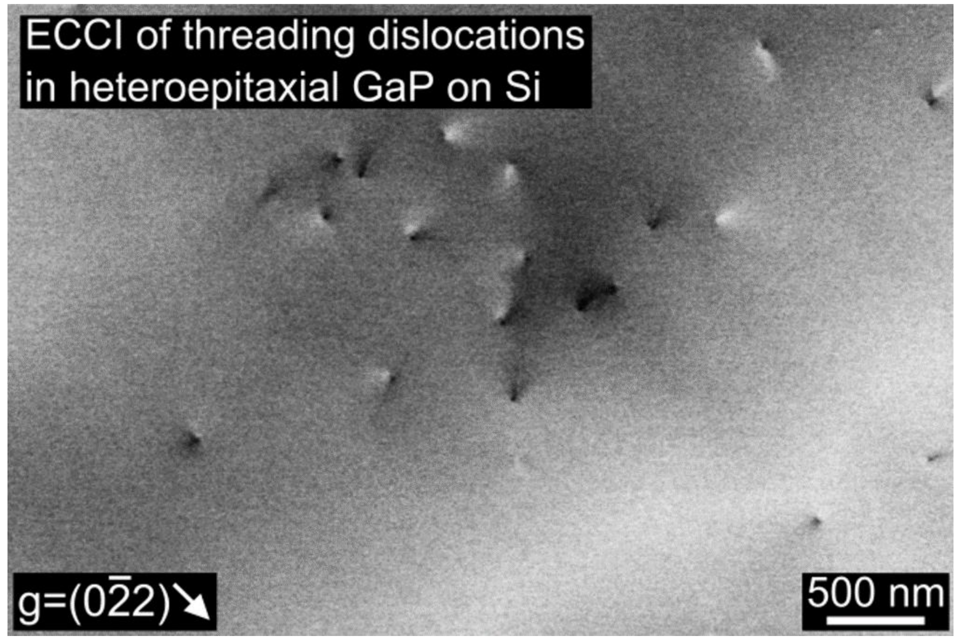
PbSe chiral branched NW



(a) (b) (c)

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

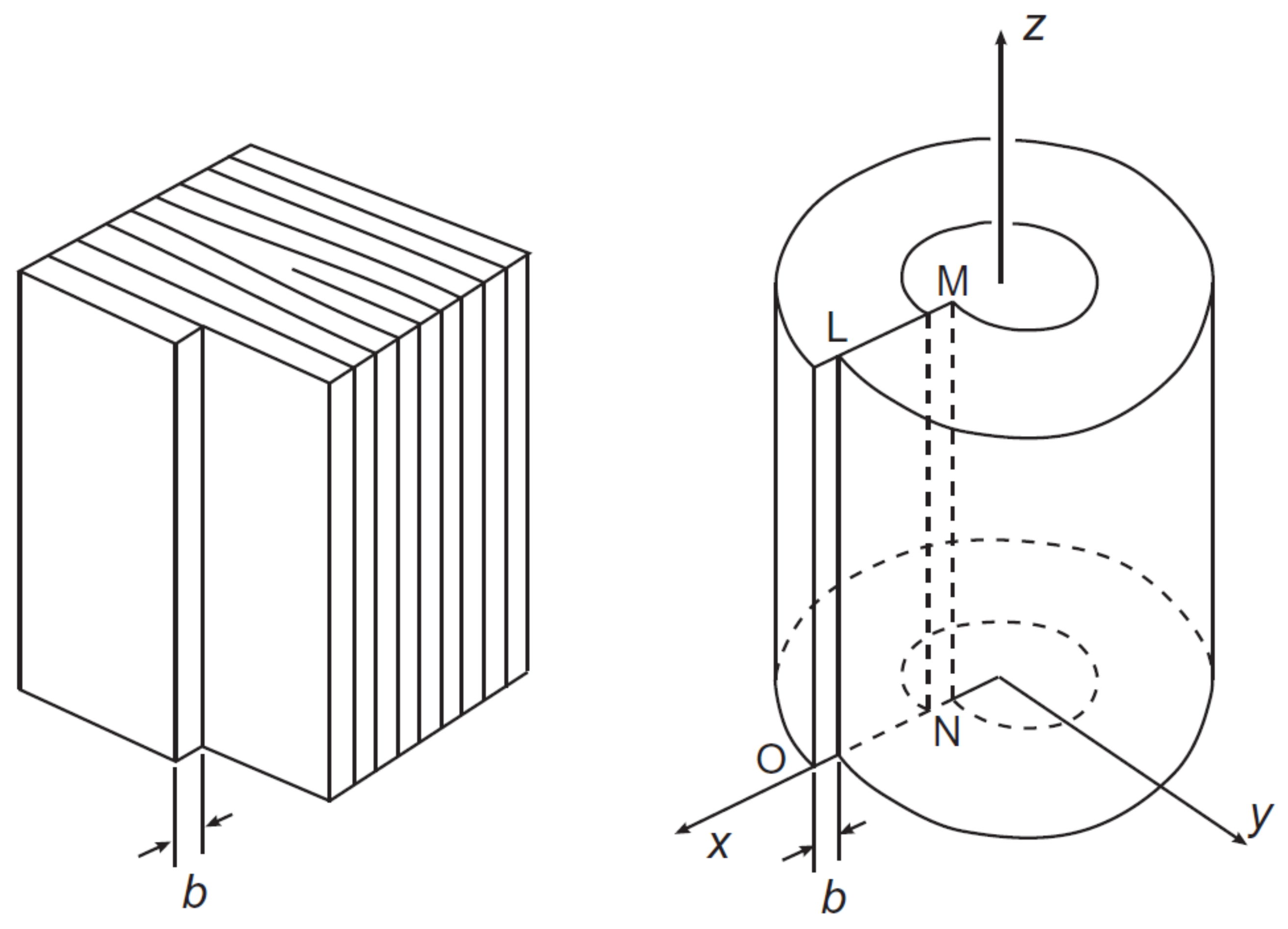
This stress produces a torque that twists the crystal around the screw dislocation.



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 (ECCI) in the scanning electron microscope.

thomas.lagrange@epfl.ch • www.epfl.ch• lumes.epfl.ch• moodle.epfl.ch• PHYS-307

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

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

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

Cylindrical Coordinates

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

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

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

Cartesian Coordinates

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

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

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

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

Elastic energy

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

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

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

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

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

Edge dislocation

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

Screw dislocation (infinite)

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

Mixed dislocation

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

Hollow core

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

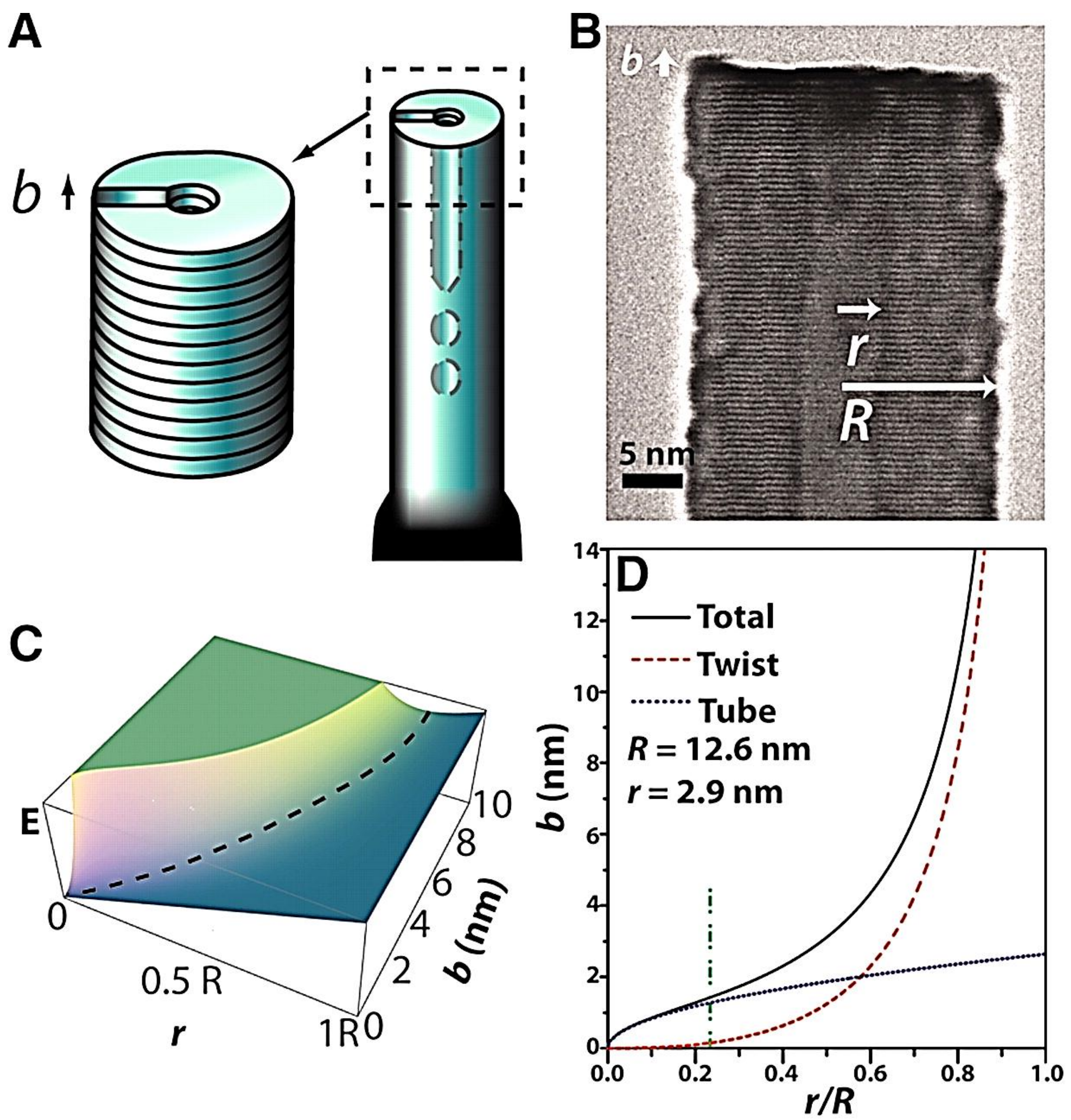
$$\left.\frac{\partial W}{\partial r}\right)_{r=r_0} = 0 \qquad r_0 = \frac{\mu b^2}{8\pi^2 \gamma}$$

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

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

Characteristics of large Burgers vectors

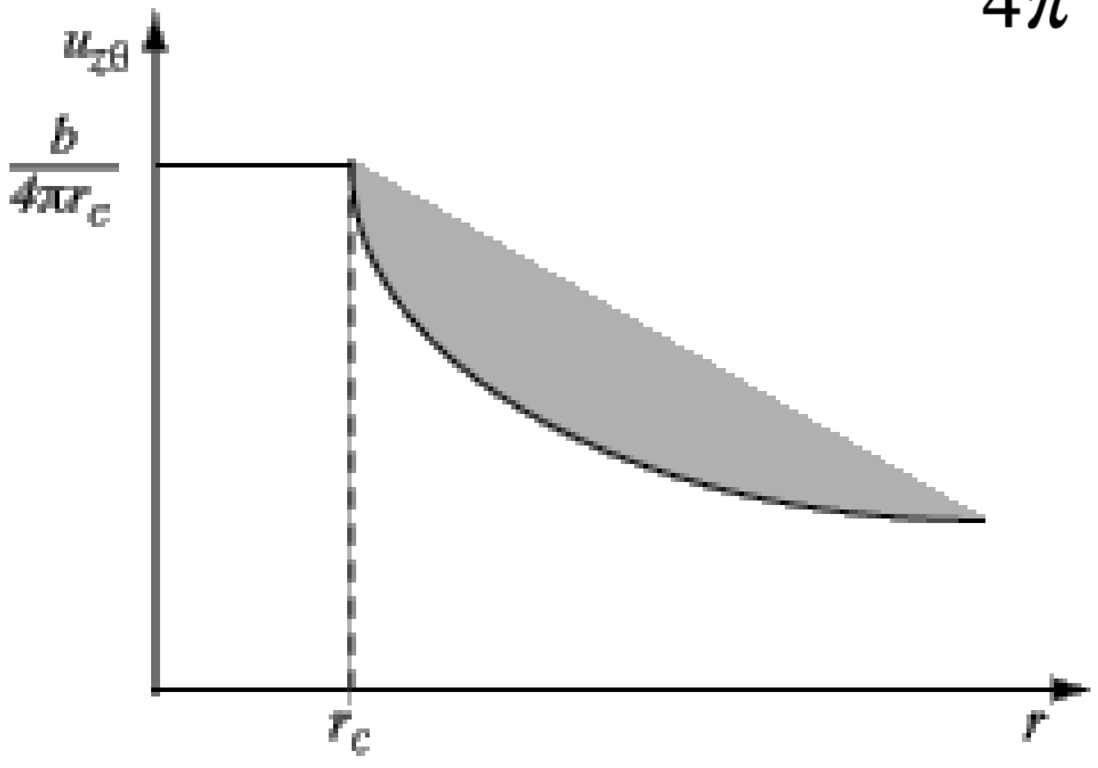
Example: Nanotubes



thomas.lagrange@epfl.ch • www.epfl.ch• lumes.epfl.ch• moodle.epfl.ch• PHYS-307

Core of a dislocation

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



Filled core

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

Screw dislocation

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

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

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

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

The interaction energy between dislocations

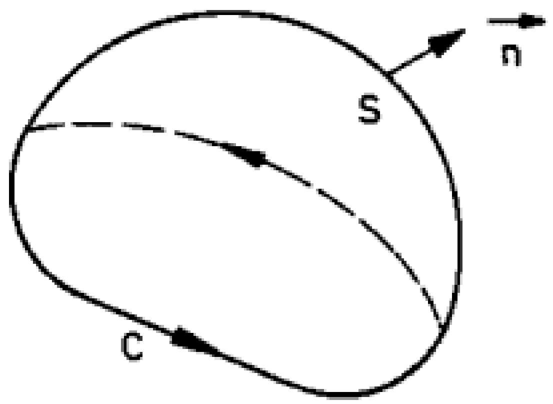
$$E = \frac{1}{2}\int_V \sigma_{ij}^A u_{ij}^A + \frac{1}{2}\int_V \sigma_{ij}^B u_{ij}^B + \frac{1}{2}\int_V \sigma_{ij}^A u_{ij}^B + \frac{1}{2}\int_V \sigma_{ij}^B u_{ij}^A$$

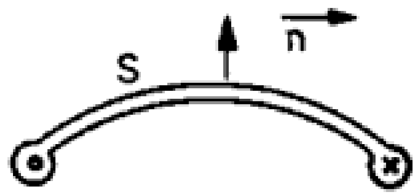
$$\frac{1}{2}\int_V \sigma_{ij}^A u_{ij}^B = \frac{1}{2}\int_V \sigma_{ij}^B u_{ij}^A$$

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

$$= 0$$

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

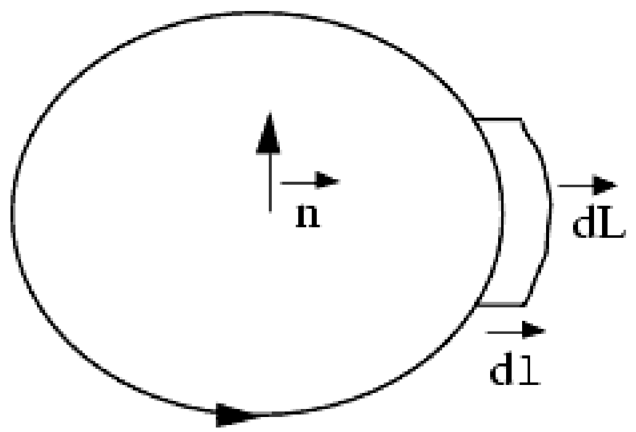




$$W_I = \int_S \sigma_{ij}^B u_i^A \, dS_j = b_i^A \int_S \sigma_{ij}^B \, dS_j = \vec{b}^A \cdot \int_S \overline{\overline{\sigma}}^B \, \overrightarrow{dS}$$

Force on a dislocation

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



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

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

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)

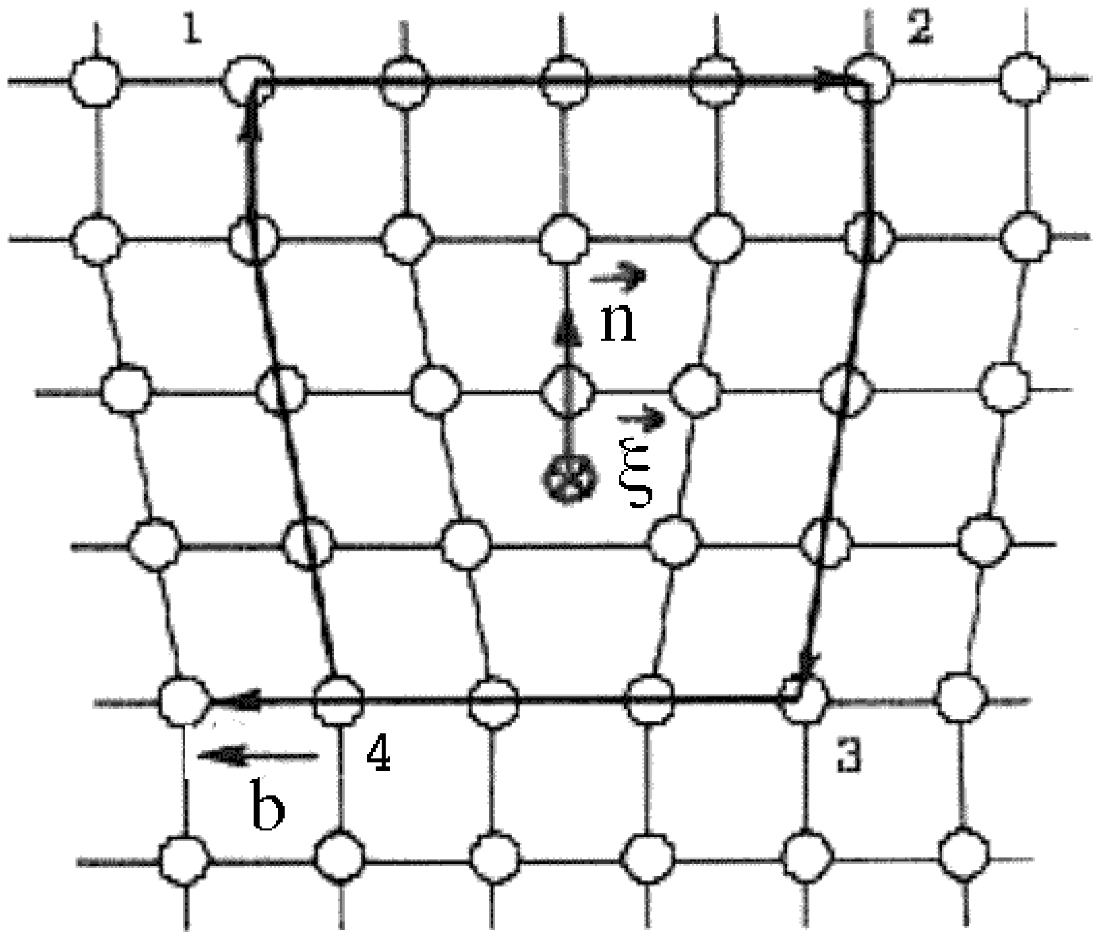
$$F_{\perp} = \left(\left(\vec{b} \cdot \bar{\bar{\sigma}}\right) \wedge \vec{\xi}\right) \cdot \vec{n}$$

b) parallel to the dislocation line

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

c) in the slip plane

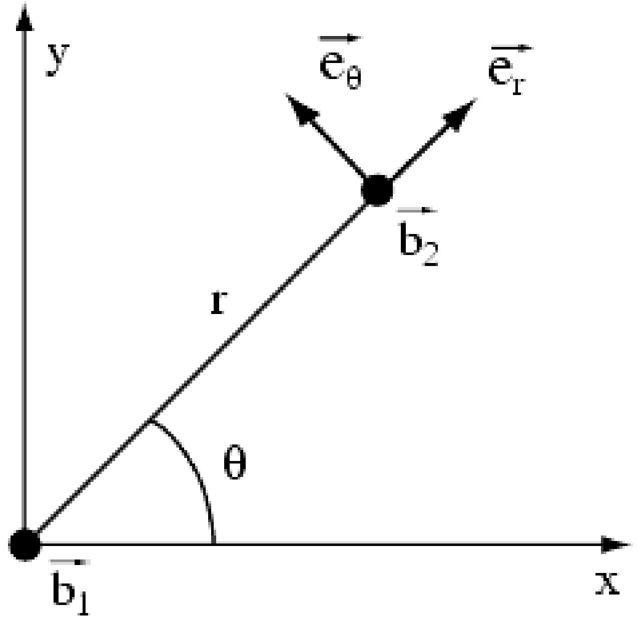
$$F_{p} = \left(\left(\vec{b} \cdot \bar{\bar{\sigma}}\right) \wedge \vec{\xi}\right) \cdot \frac{\vec{b}}{|b|} = \left(\vec{b} \cdot \bar{\bar{\sigma}}\right) \cdot \vec{n}$$



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

Interaction between dislocations

Two parallel screw dislocations



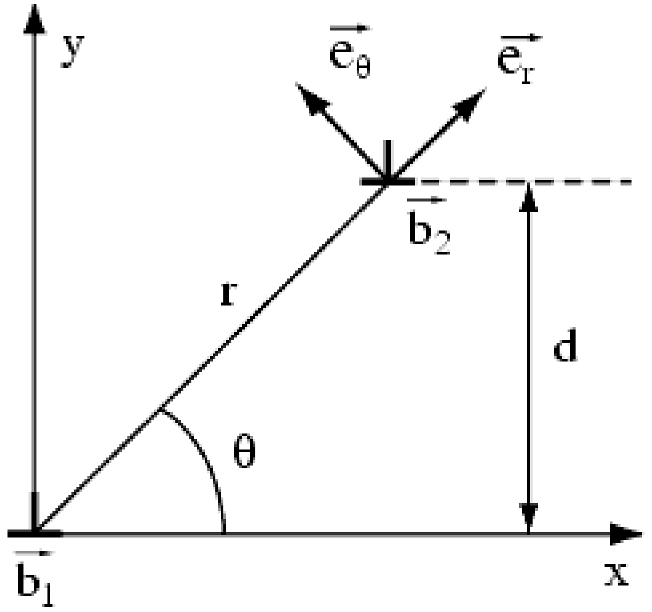
$$\vec{b}_1 = (0,0,b_1)$$

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

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

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

Two parallel edge dislocations



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

$$\vec{b}_1 = (b_2,0,0,)$$

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

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

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

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

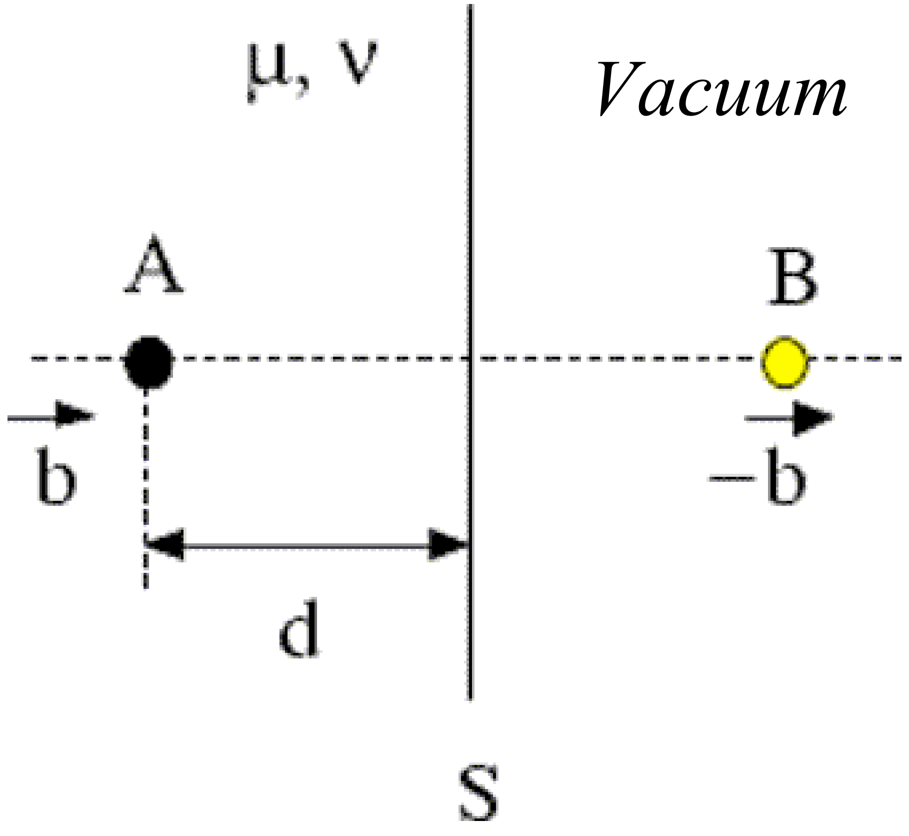
$$F_x = \frac{\mu b_1 b_2}{2\pi(1-\nu)} \frac{\cos\theta\cos 2\theta}{r}$$

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

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

thomas.lagrange@epfl.ch • www.epfl.ch• lumes.epfl.ch• moodle.epfl.ch• PHYS-307

Surface forces



Self-energy

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

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

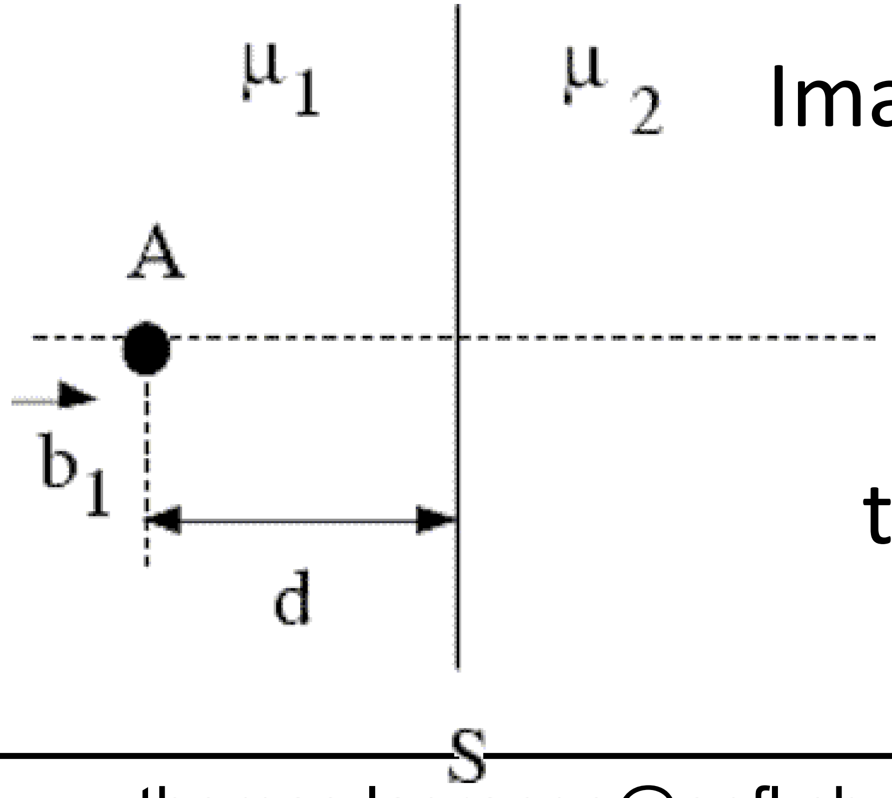
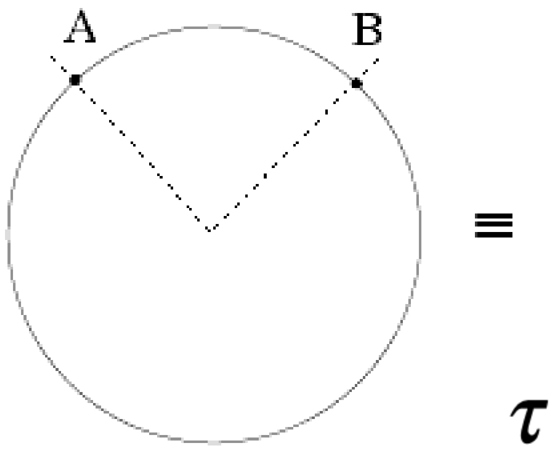
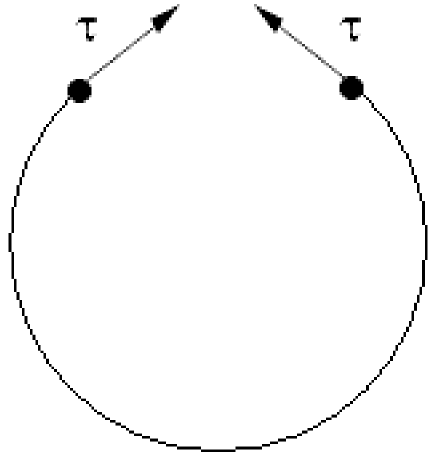


Image force for screw dislocation $F = \frac{\mu b^2}{4\pi d}$

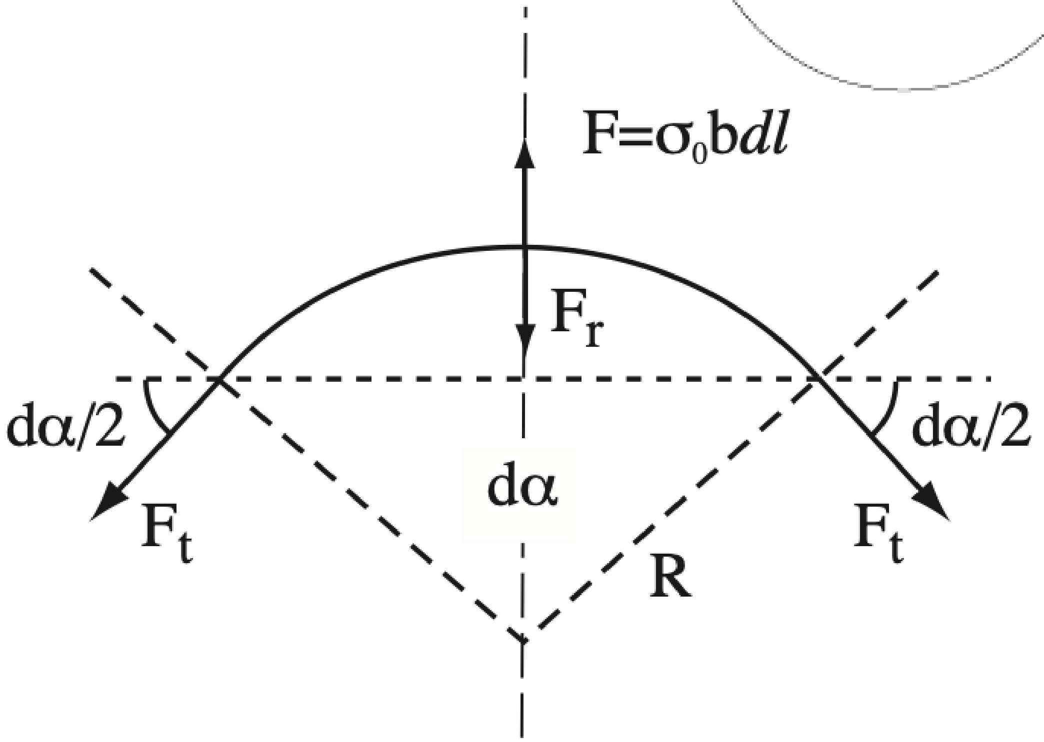
Two environments of different modulus:
the environment with the weaker modulus
attracts the dislocation

Line tension





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



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

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

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

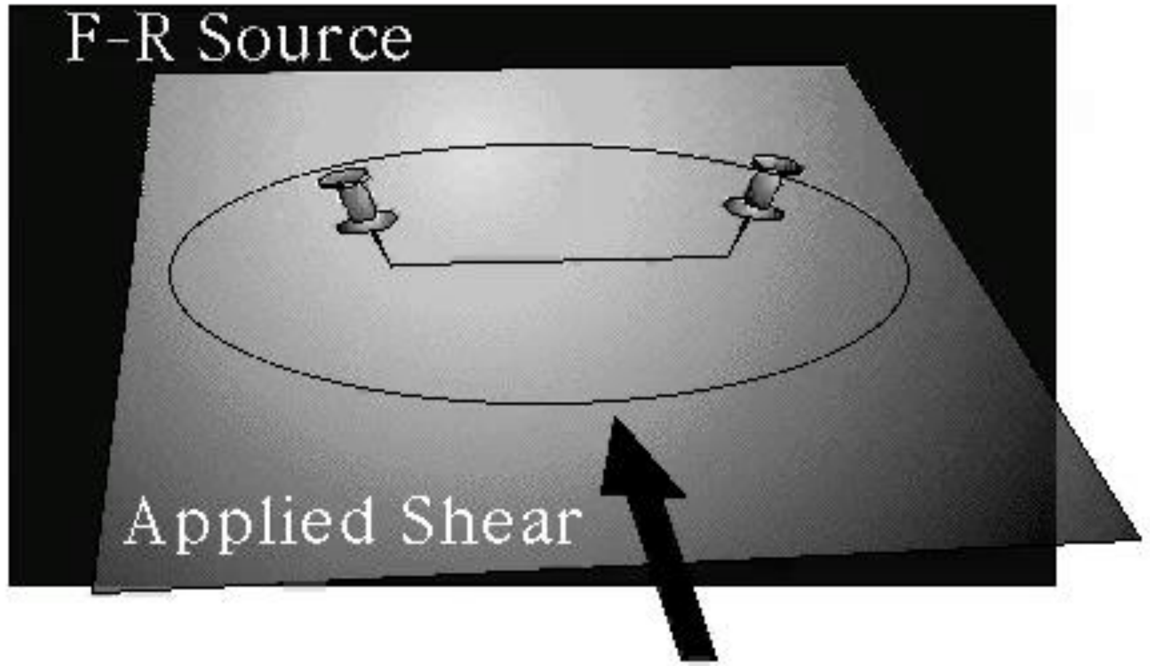
$$W[J/m] = \frac{\mu b^2}{4\pi K}\ln\frac{R}{b} \rightarrow dW[J] = \frac{\mu b^2}{4\pi K}\ln\frac{R}{b}dl$$

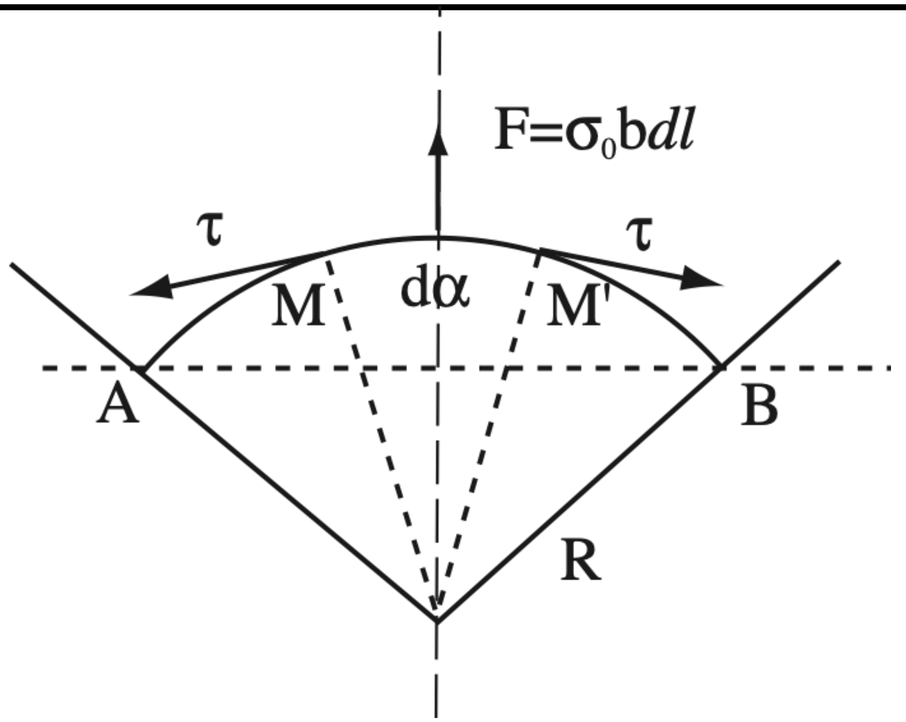
$$K = \frac{1-\nu}{1-\nu\cos^2\psi}$$

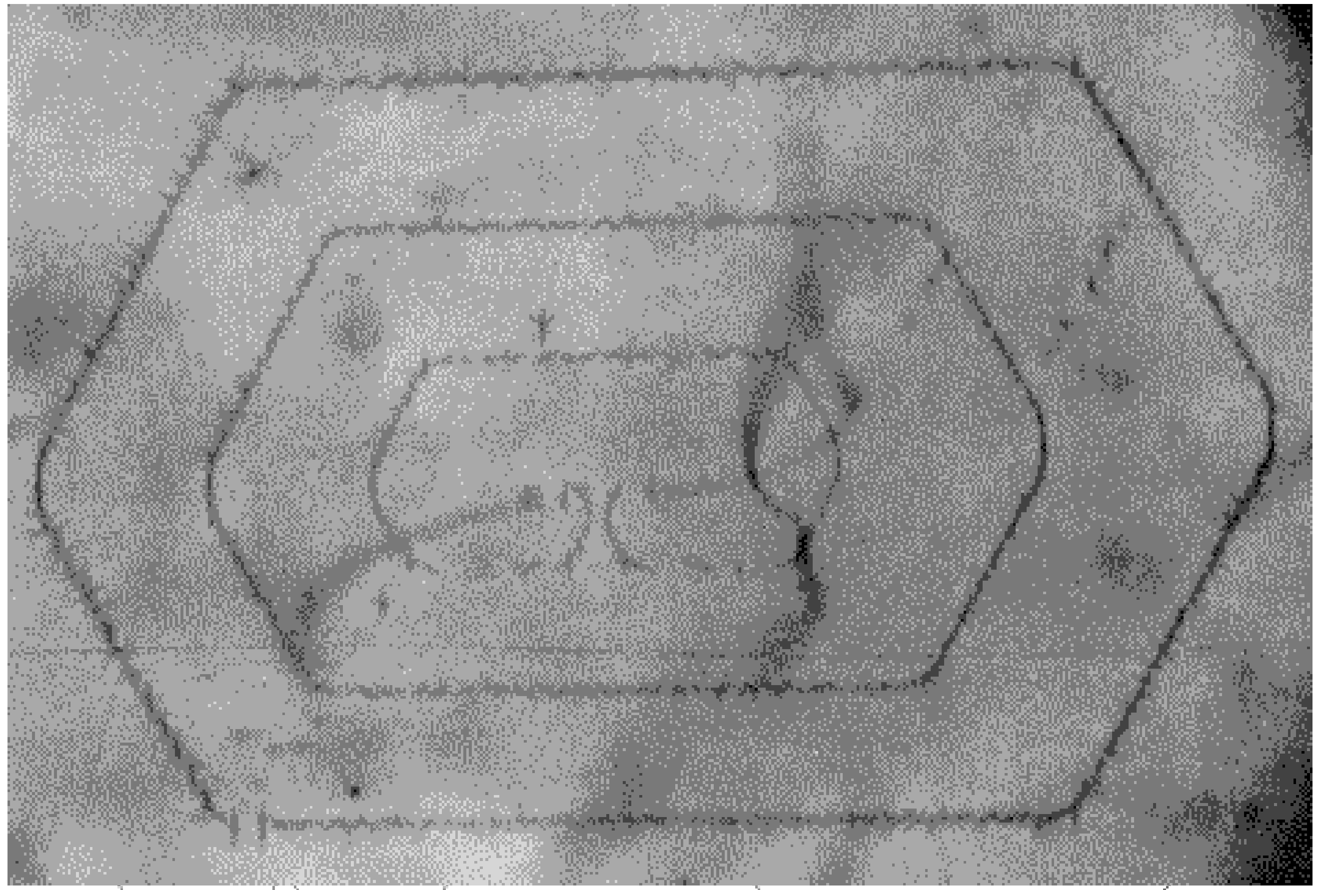
$$\boxed{\tau[N] = \frac{\mu b^2}{4\pi K}\ln\frac{R}{b}} \approx \mu b^2$$

thomas.lagrange@epfl.ch • www.epfl.ch• lumes.epfl.ch• moodle.epfl.ch• PHYS-307

Application of the line tension: Frank Read source







$$2\tau\sin(d\alpha/2) = \sigma_0 b dl = \sigma_0 b R d\alpha$$

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

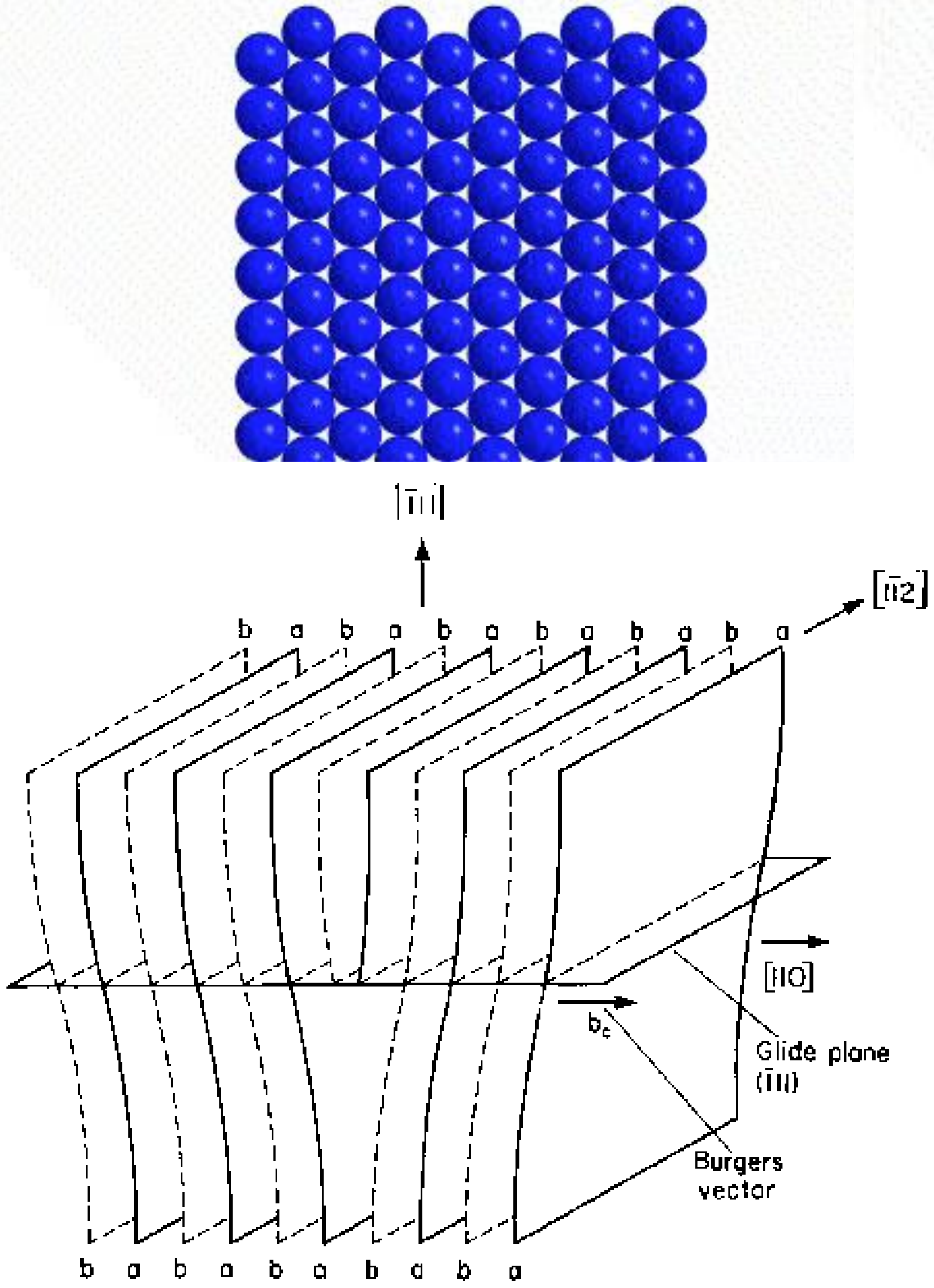
$$\sigma_0 = \frac{2\tau}{bl} \approx \frac{\mu b}{l} \sim 2.5\cdot 10^{-5}\mu$$

$\sigma_0 \sim 2.4$ MPa for copper

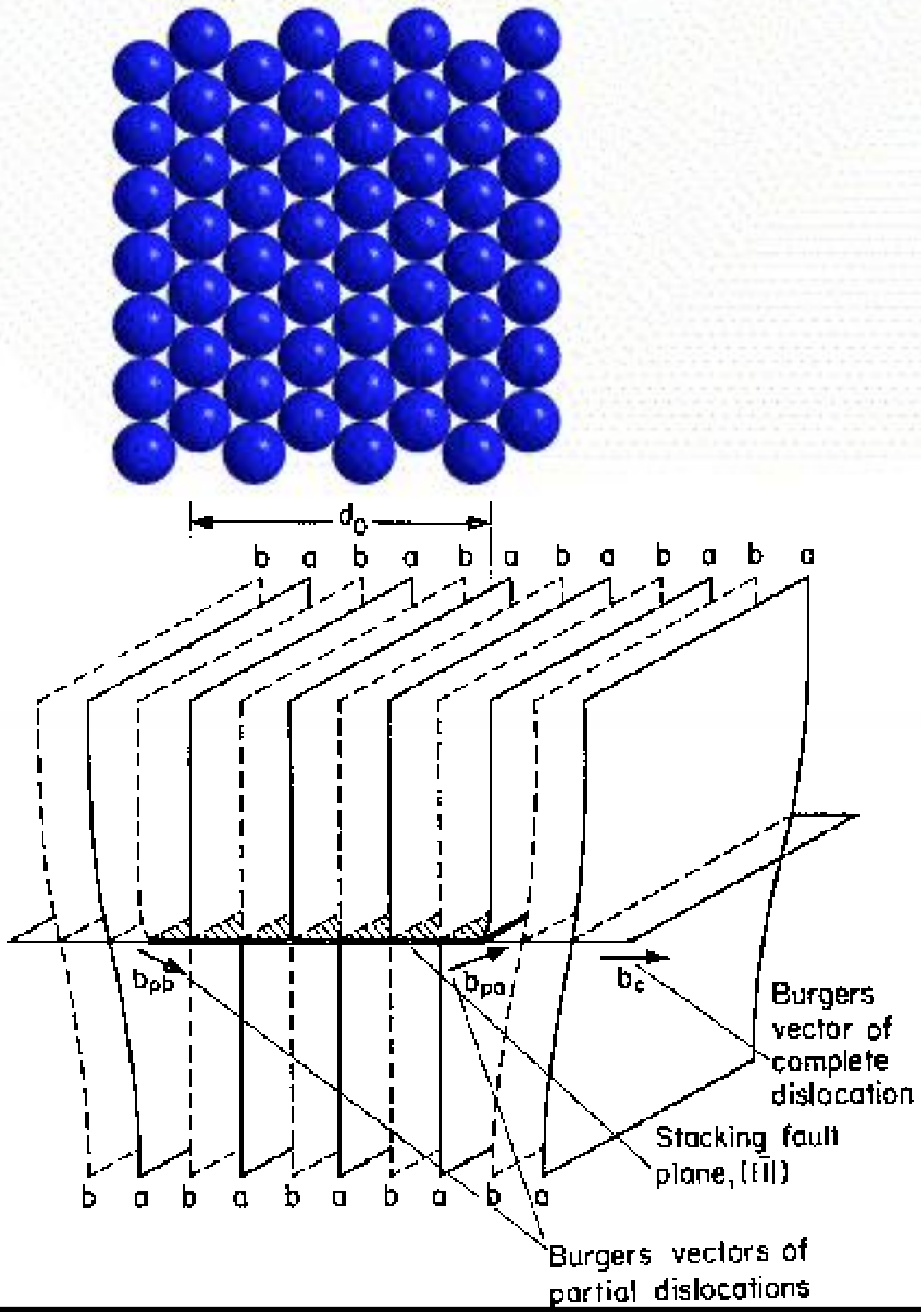
thomas.lagrange@epfl.ch • www.epfl.ch• lumes.epfl.ch• moodle.epfl.ch• PHYS-307

Dislocations in face-centered cubic metals

FCC

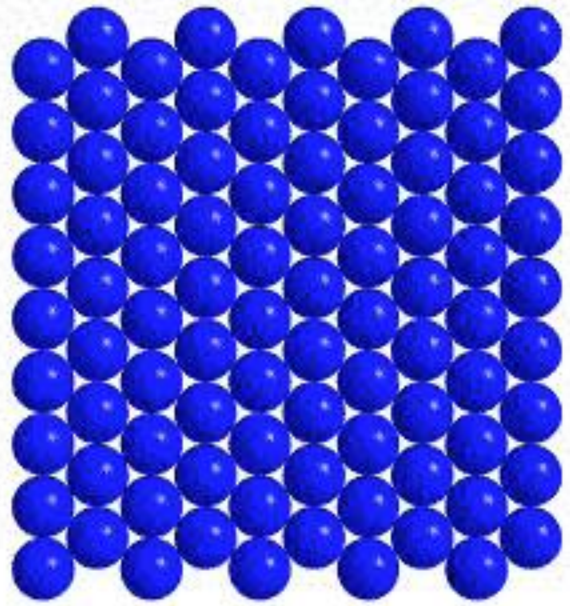


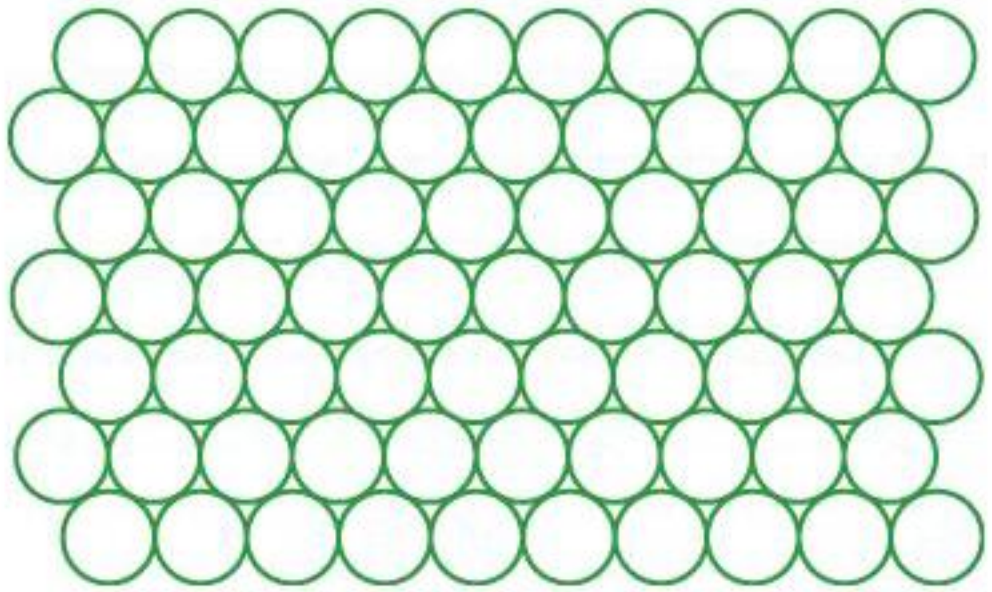
HCP



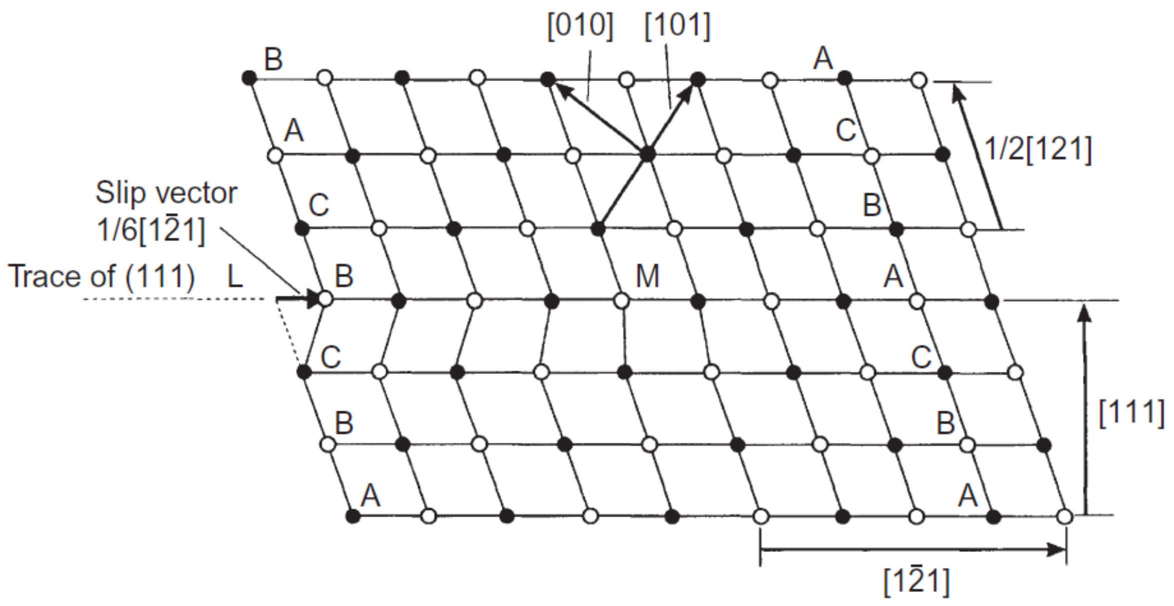
Dislocations in face-centered cubic metals

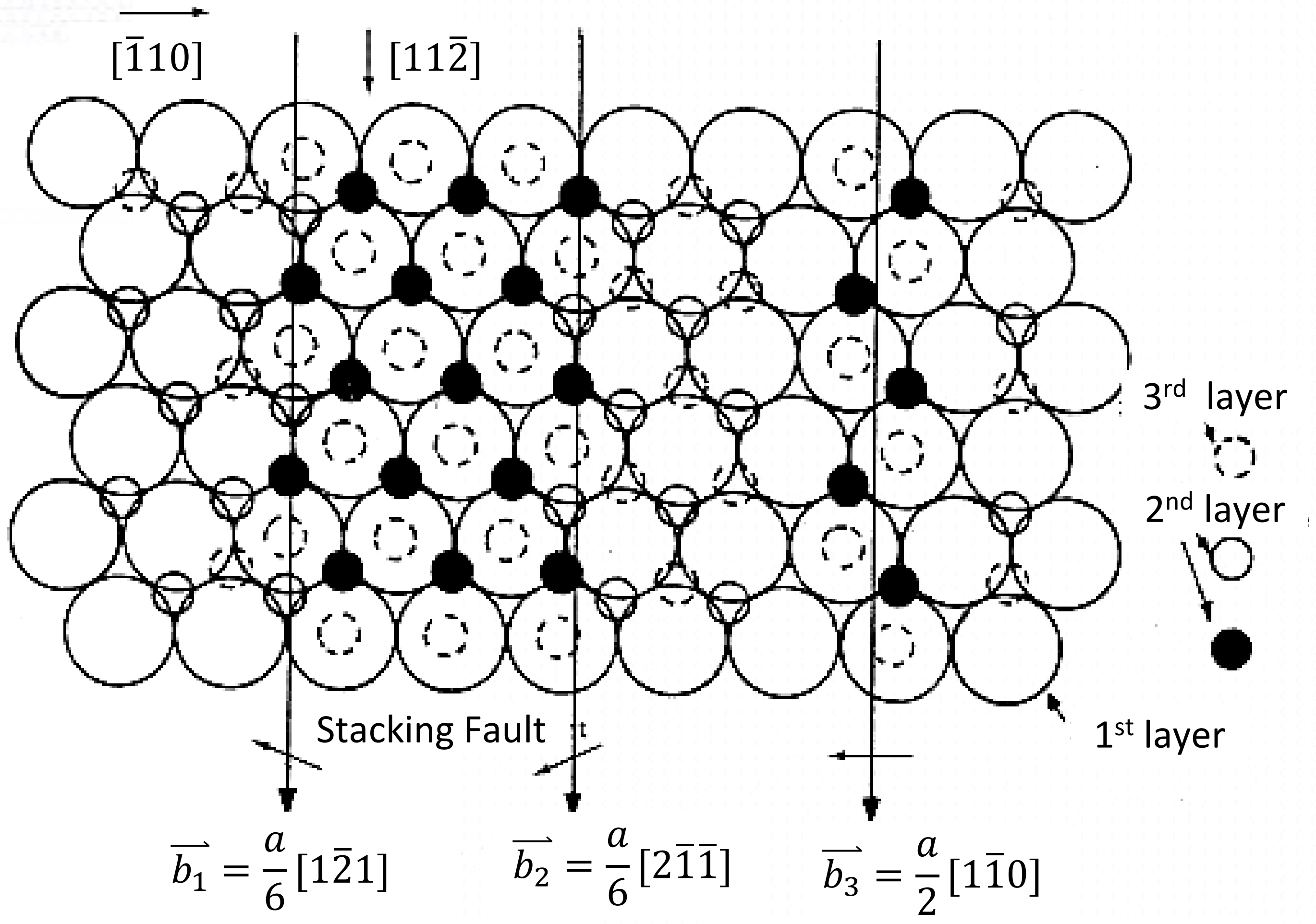
FCC



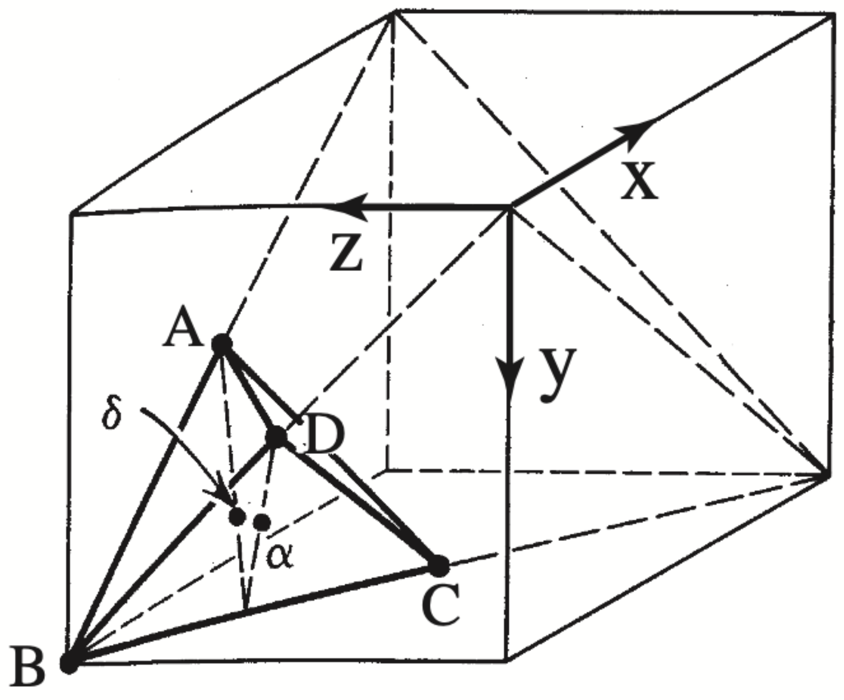


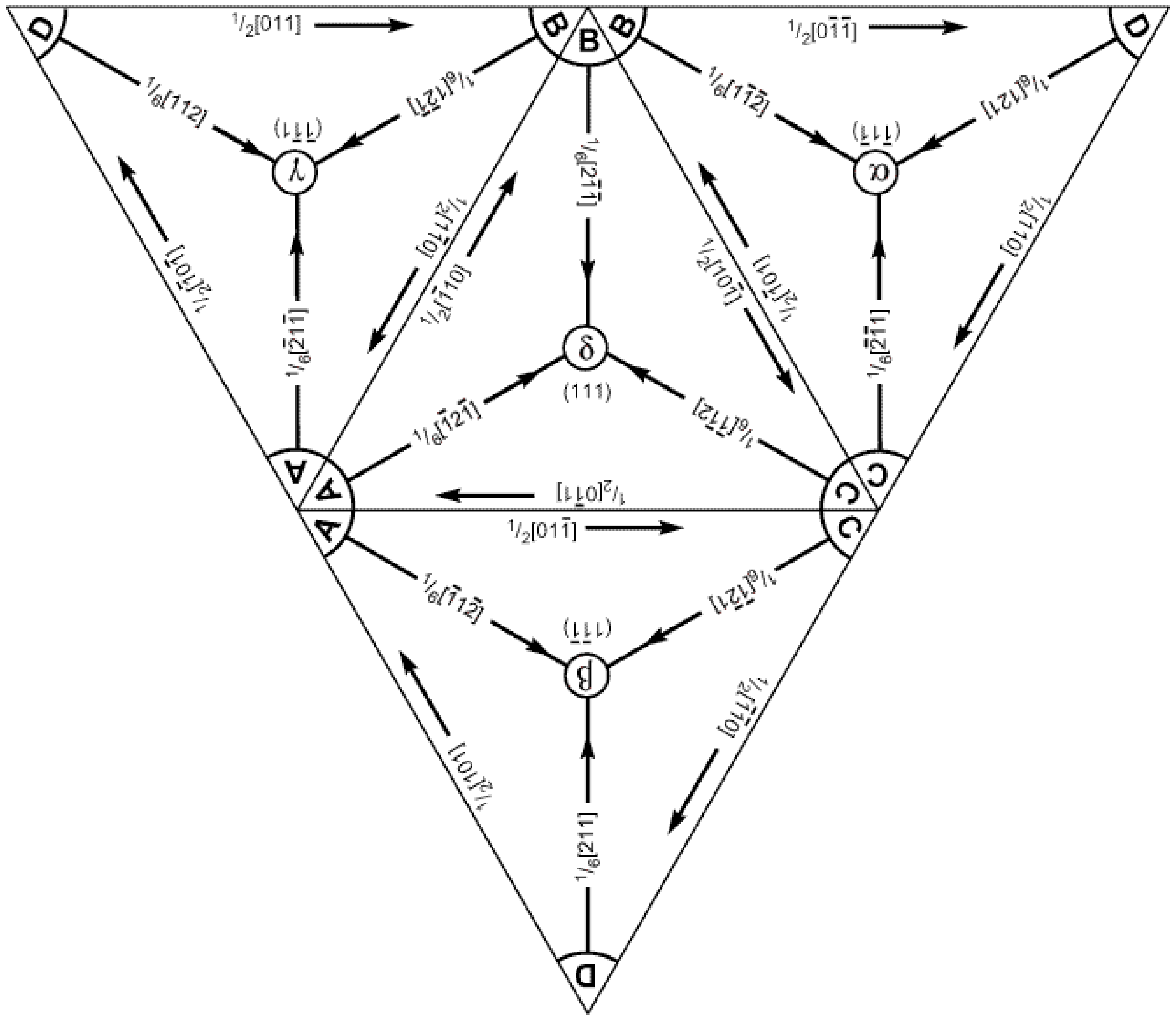
Shockley partial





Thompson tetrahedron

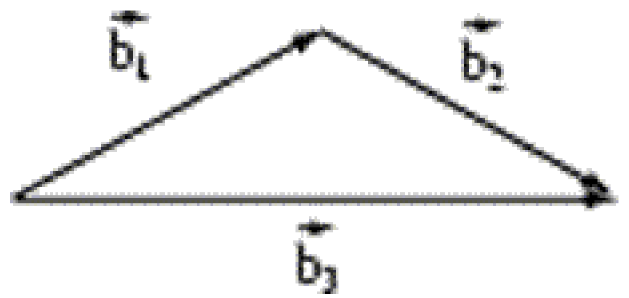




Energy calculation

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

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



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

Frank's Rule

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

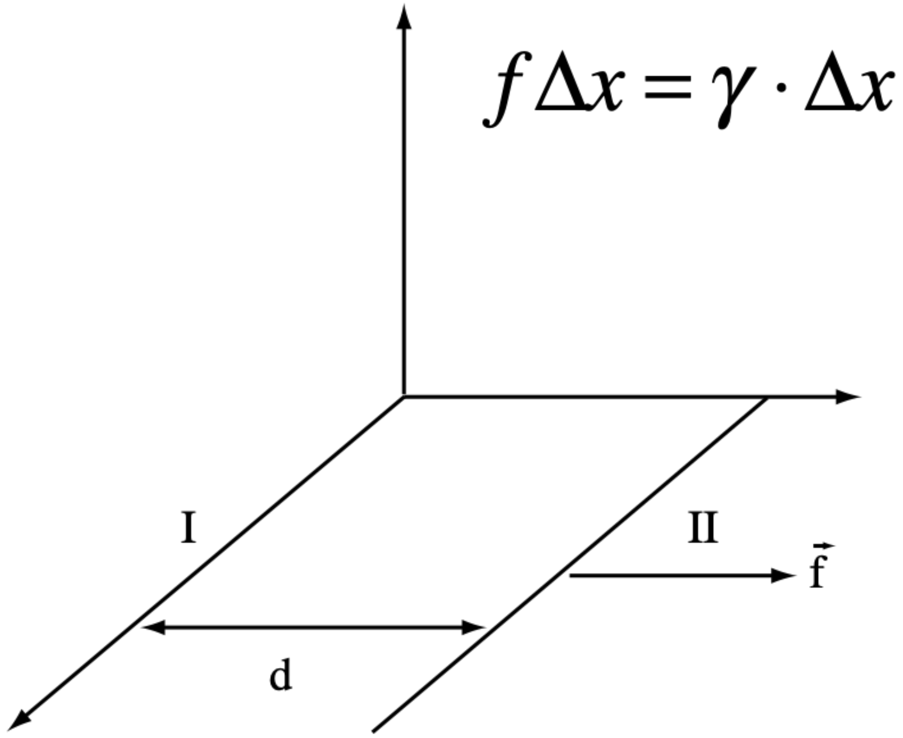
Dislocation dissociates into partials

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

Dislocation does not dissociate into partials

thomas.lagrange@epfl.ch • www.epfl.ch• lumes.epfl.ch• moodle.epfl.ch• PHYS-307

Energy of stacking fault



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

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

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

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

applications

Copper: $\boldsymbol{\mu}$ = 4.85 x10^4 J cm^{-3} $\boldsymbol{\gamma}$= 4 μJ cm^{-2}

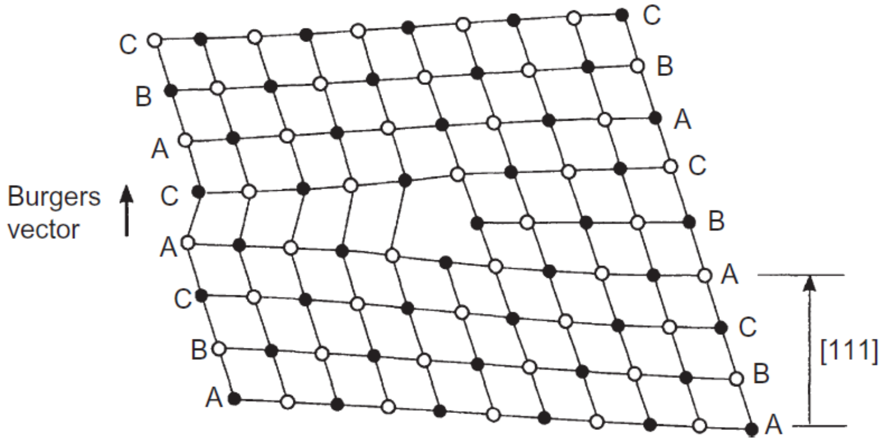
a = 3.62x10^{-8} cm $\boldsymbol{\nu}$ = 0.33 d = 3.7 nm

Aluminum: $\boldsymbol{\mu}$ = 2.8x10^4 J cm^{-3} $\boldsymbol{\gamma}$= 20 μJ cm^{-2}

a = 4.05x10^{-8} cm $\boldsymbol{\nu}$ = 0.33 d = 0.54 nm

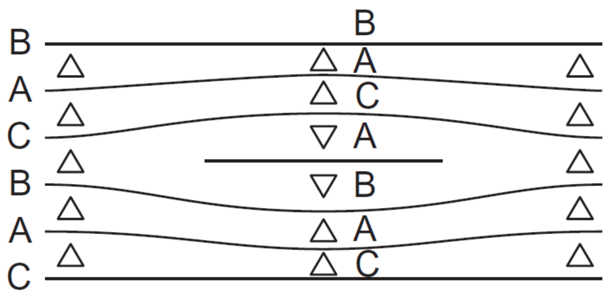
Sessile dislocations

Frank partial dislocation

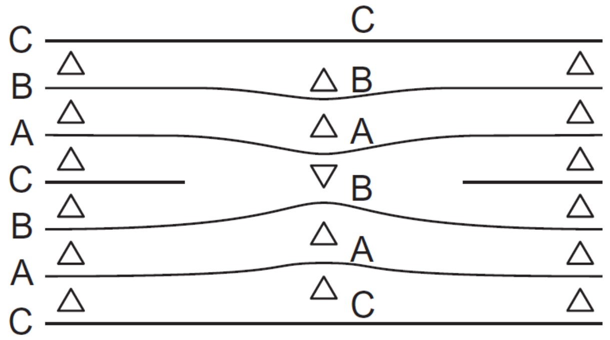


$$\vec{b} = \overrightarrow{A\alpha} = \frac{a}{3}[\bar{1}1\bar{1}]$$

Positive Frank dislocation (extrinsic stacking fault)

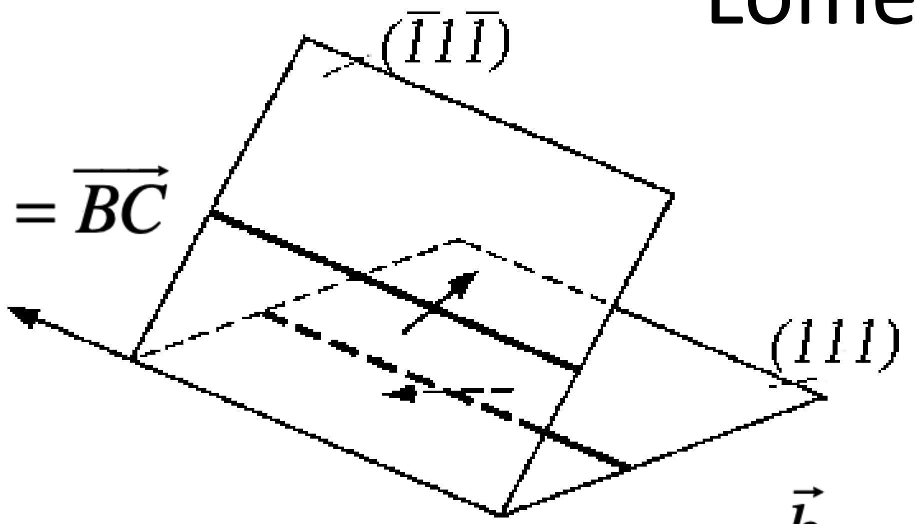


Negative Frank dislocation (intrinsic stacking fault)



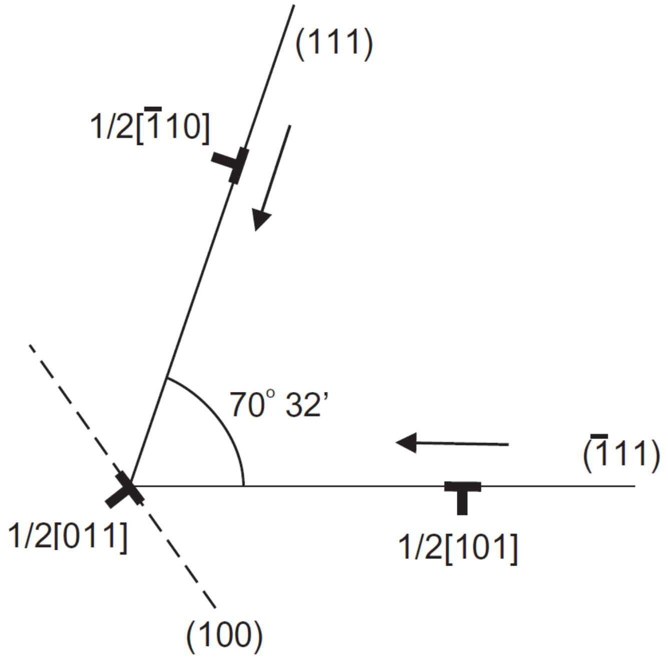
Lomer dislocation

$$\vec{b}_a = \frac{a}{2}[10\bar{1}] = \overrightarrow{BC}$$



$$\vec{b}_b = \frac{a}{2}[0\bar{1}1] = \overrightarrow{CA}$$

$$\overrightarrow{BA} = \overrightarrow{BC} + \overrightarrow{CA} = \frac{a}{2}[1\bar{1}0]$$

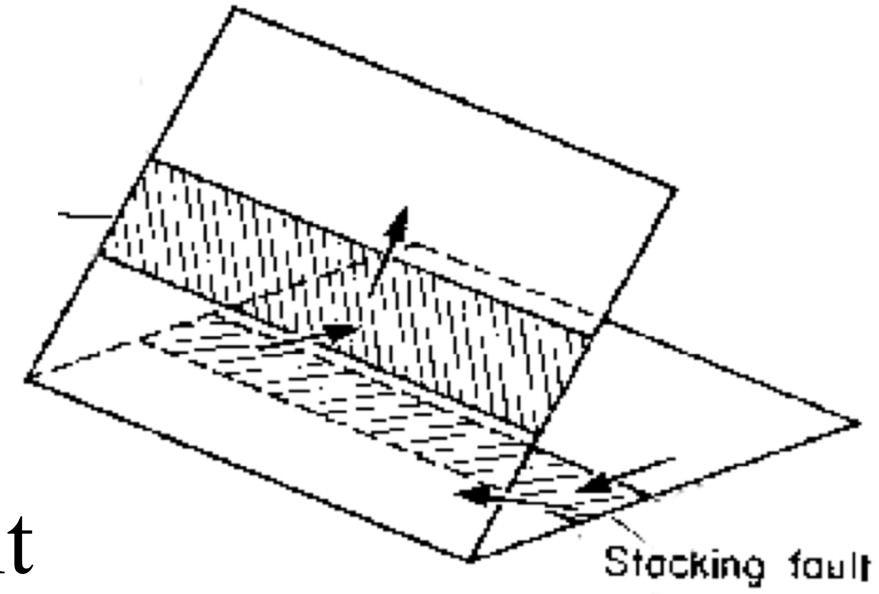


thomas.lagrange@epfl.ch • www.epfl.ch• lumes.epfl.ch• moodle.epfl.ch• PHYS-307

Sessile dislocations

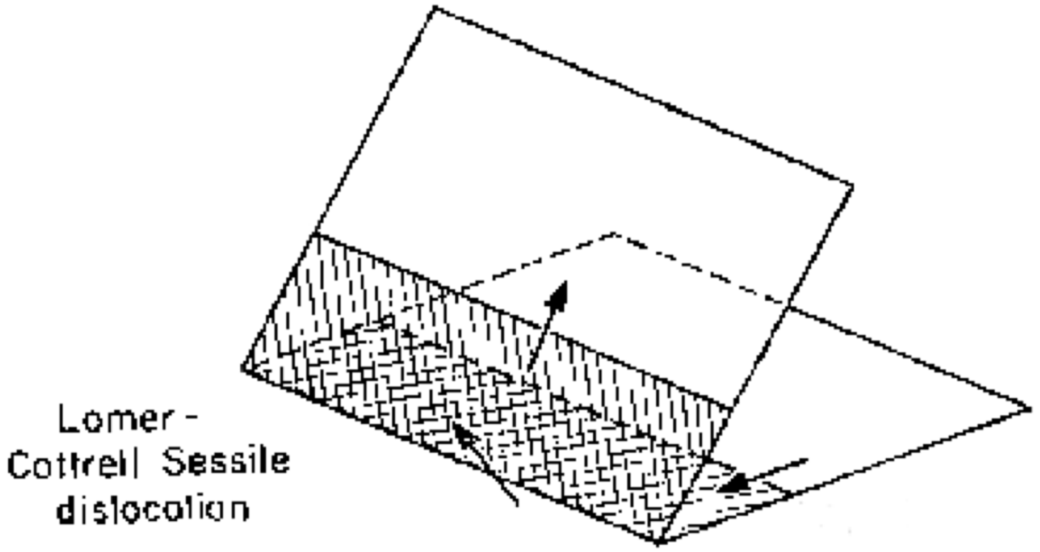
Lomer Cottrell dislocation

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



Stacking fault

$$\overrightarrow{BC} = \overrightarrow{B\alpha} + \overrightarrow{\alpha C} = \frac{a}{6}[1\,\bar{1}\,\bar{2}] + \frac{a}{6}[2\,1\,\bar{1}] = \frac{a}{2}[1\,0\,\bar{1}]$$



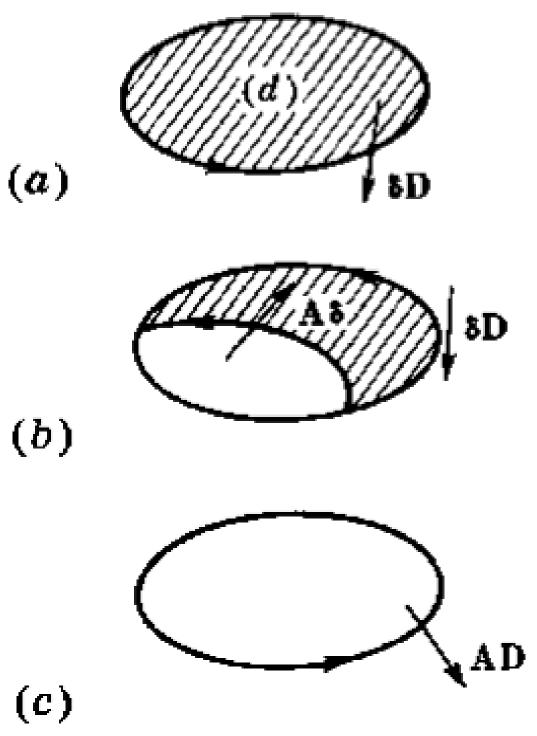
$$\overrightarrow{\alpha\beta} = \overrightarrow{\alpha C} + \overrightarrow{C\beta} = \frac{a}{6}[2\,1\,\bar{1}] + \frac{a}{6}[\bar{1}\,\bar{2}\,1] = \frac{a}{6}[1\,\bar{1}\,0]$$

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

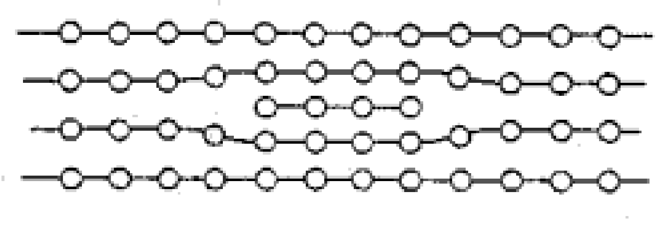
$$\frac{1}{6}[21\bar{1}] + \frac{1}{6}[\bar{1}\bar{2}1] + \frac{1}{6}[1\bar{1}0] = \frac{1}{2}\,[1\bar{1}0] \rightarrow \frac{a^2}{6} + \frac{a^2}{6} + \frac{a^2}{18} < \frac{a^2}{2}$$

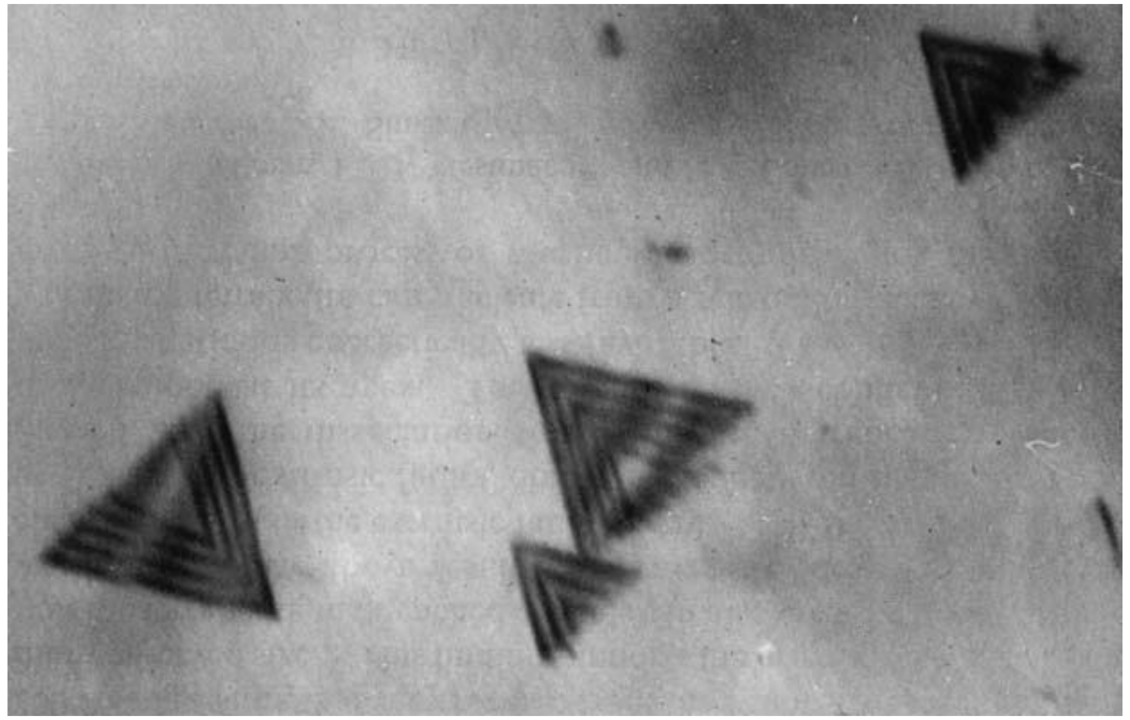
thomas.lagrange@epfl.ch • www.epfl.ch• lumes.epfl.ch• moodle.epfl.ch• PHYS-307

Prismatic loops



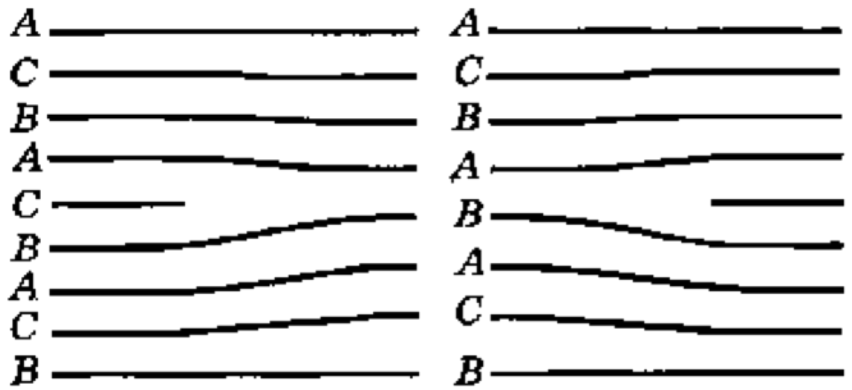
Al

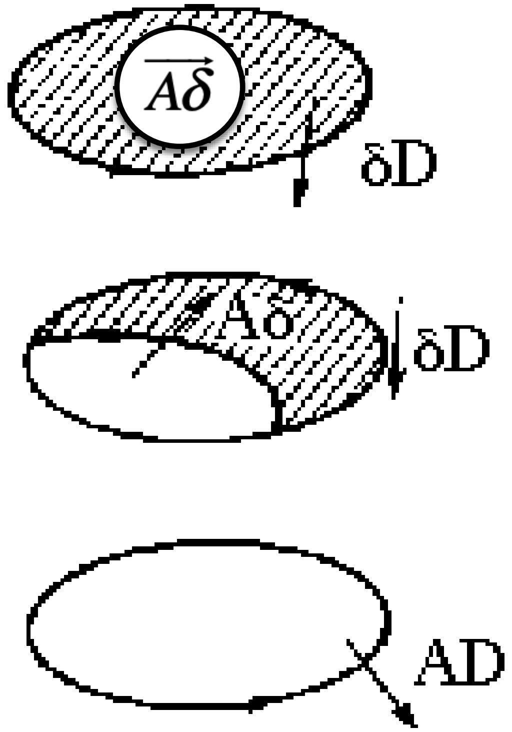




Au

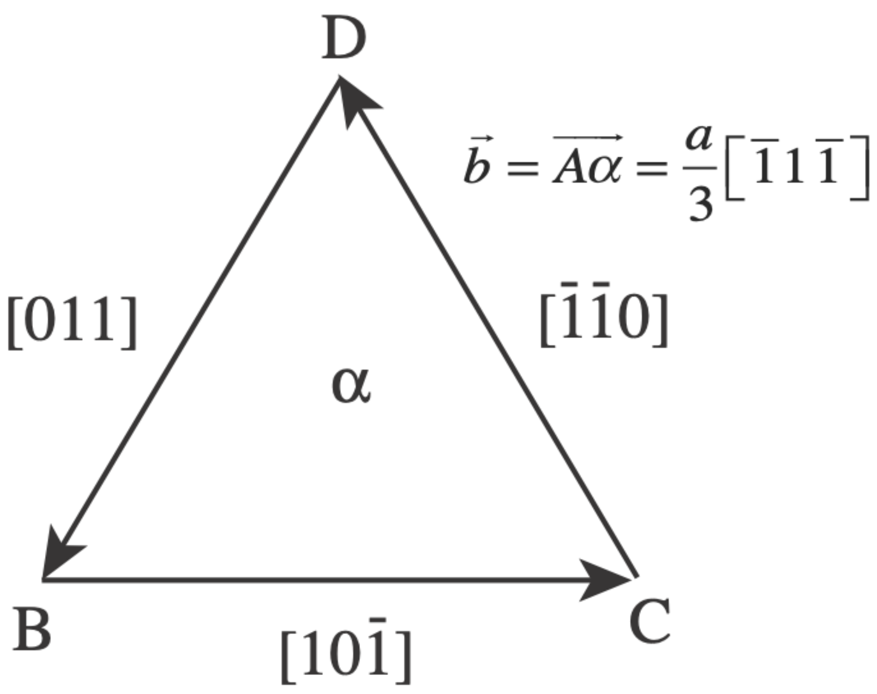
Prismatic loops





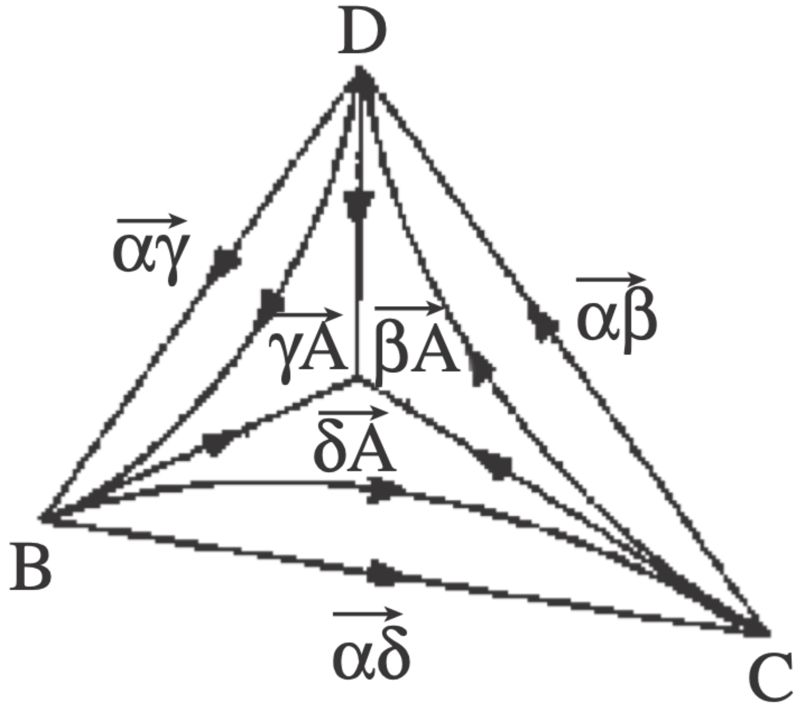
$$\overrightarrow{A\delta}+\overrightarrow{\delta D}=\overrightarrow{AD}=\frac{a}{2}[\bar{1}0\bar{1}]$$

Al: high fault energy



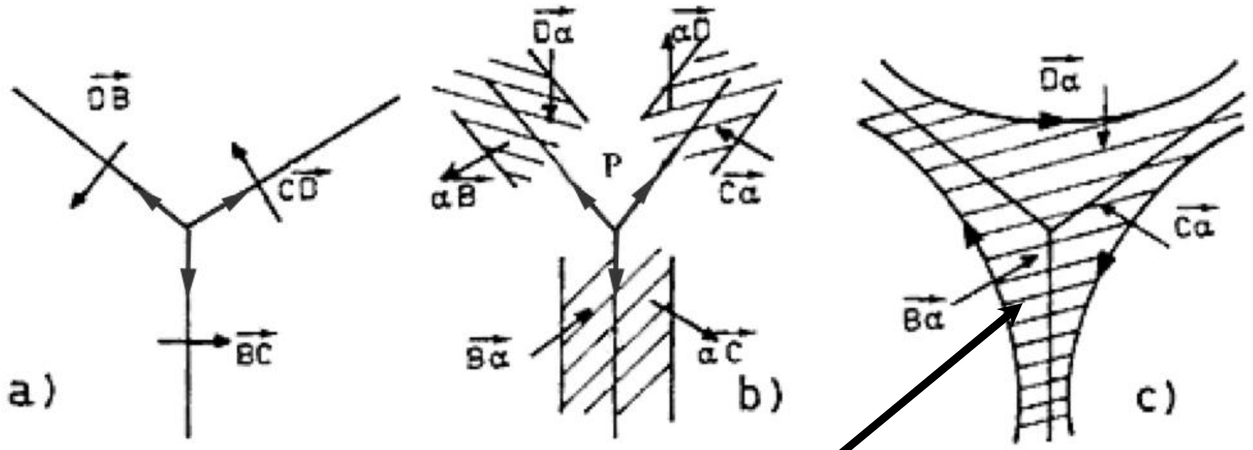
$$\frac{1}{3}[\bar{1}1\bar{1}]=\frac{1}{6}[\bar{1}2\bar{1}]+\frac{1}{6}[\bar{1}0\bar{1}]$$

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

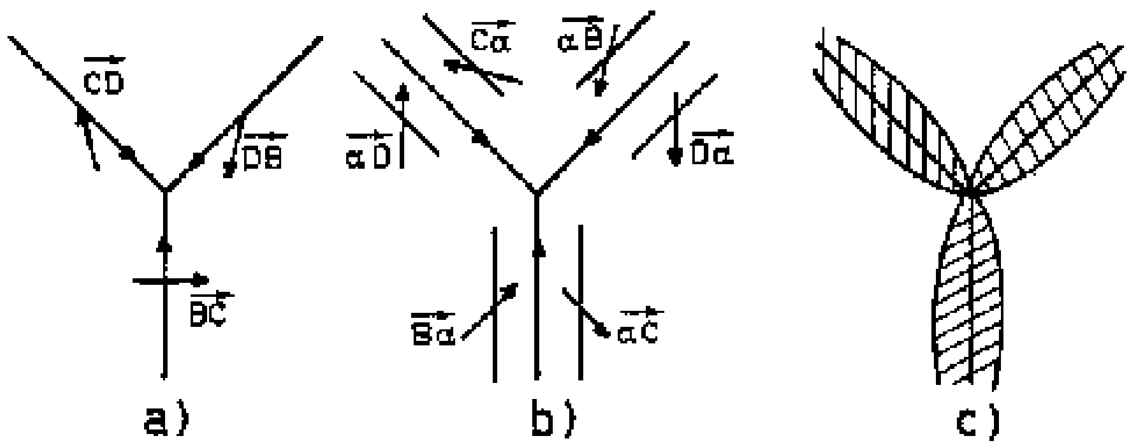


Au: low fault energy

Dislocation nodes in FCC metals



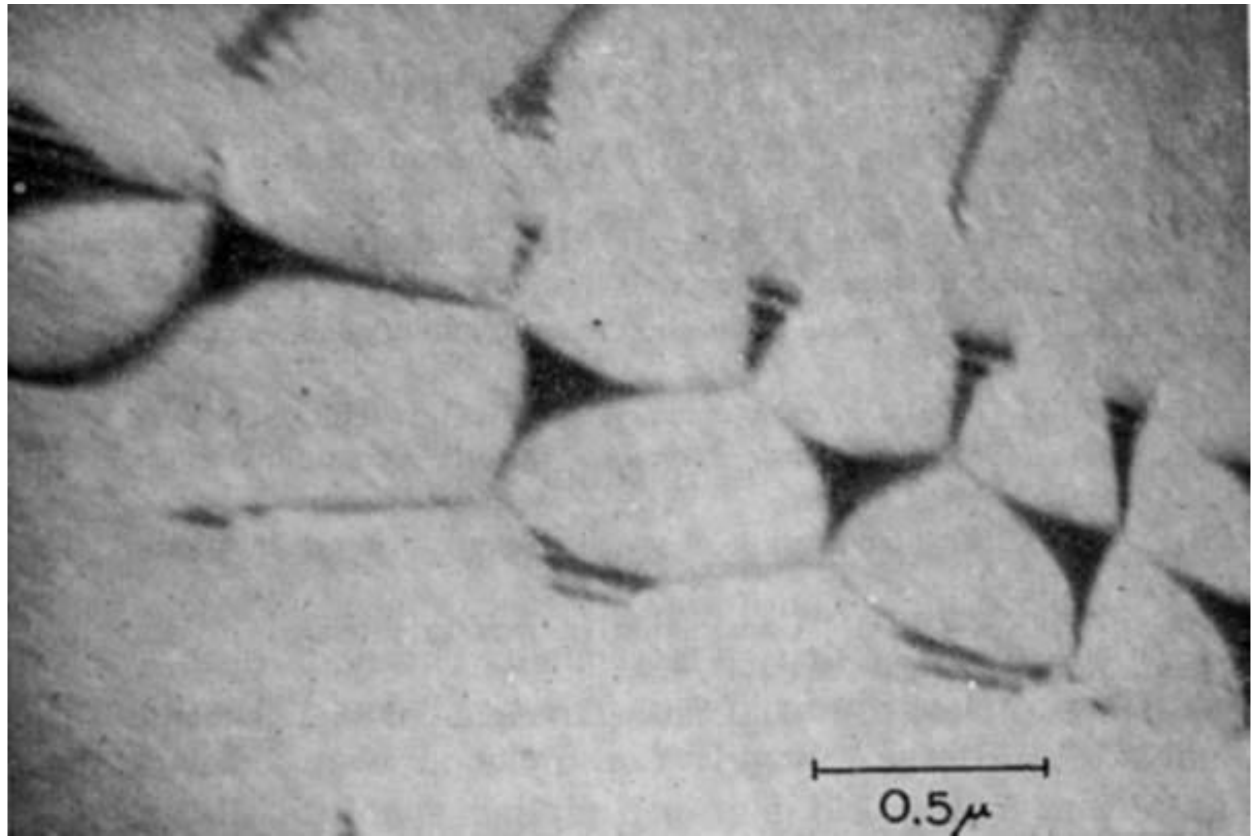
Extended



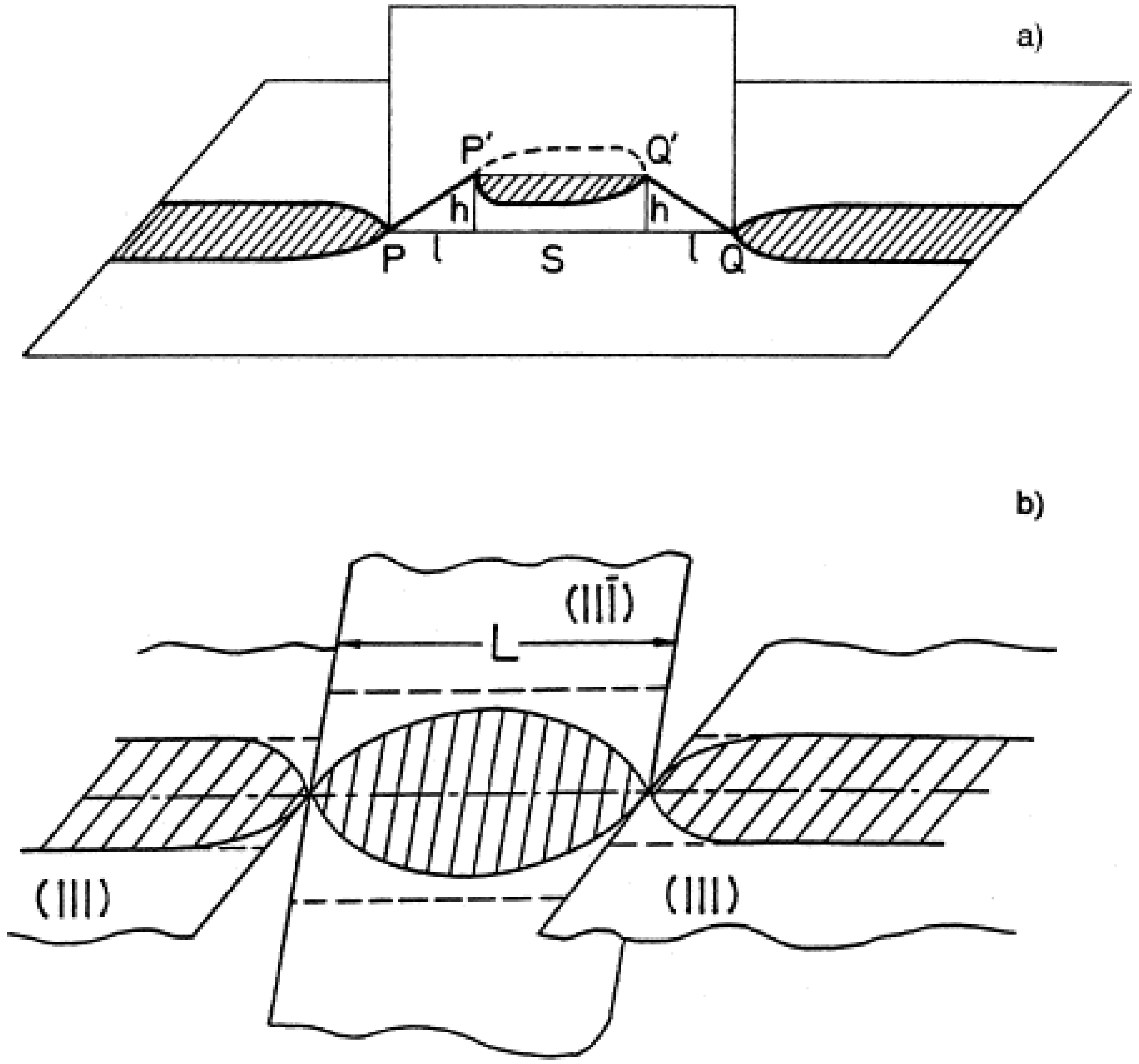
Contracted

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

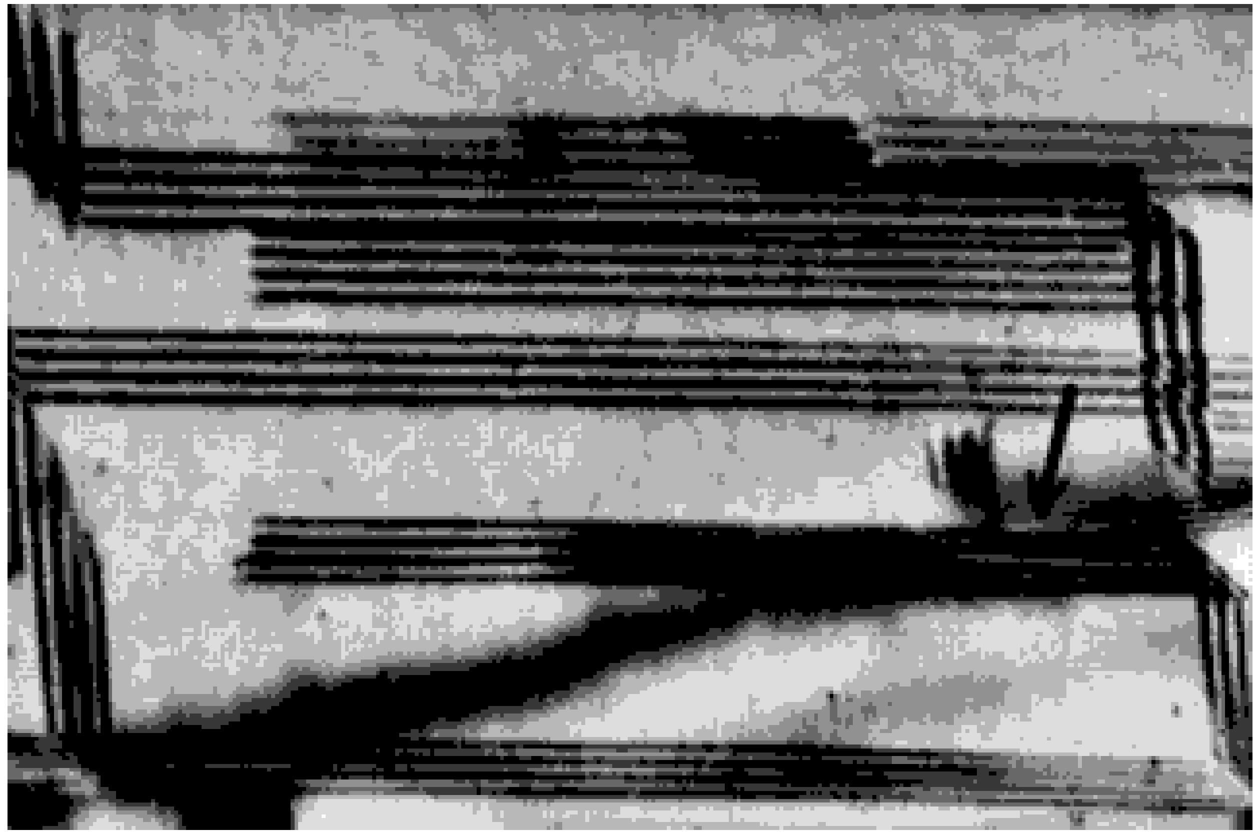
$$\gamma = \frac{\alpha \mu b_S^2}{R}$$



Cross slip in FCC metals



Stair-Rod Dislocations



Cu-10%Fe

thomas.lagrange@epfl.ch • www.epfl.ch• lumes.epfl.ch• moodle.epfl.ch• PHYS-307