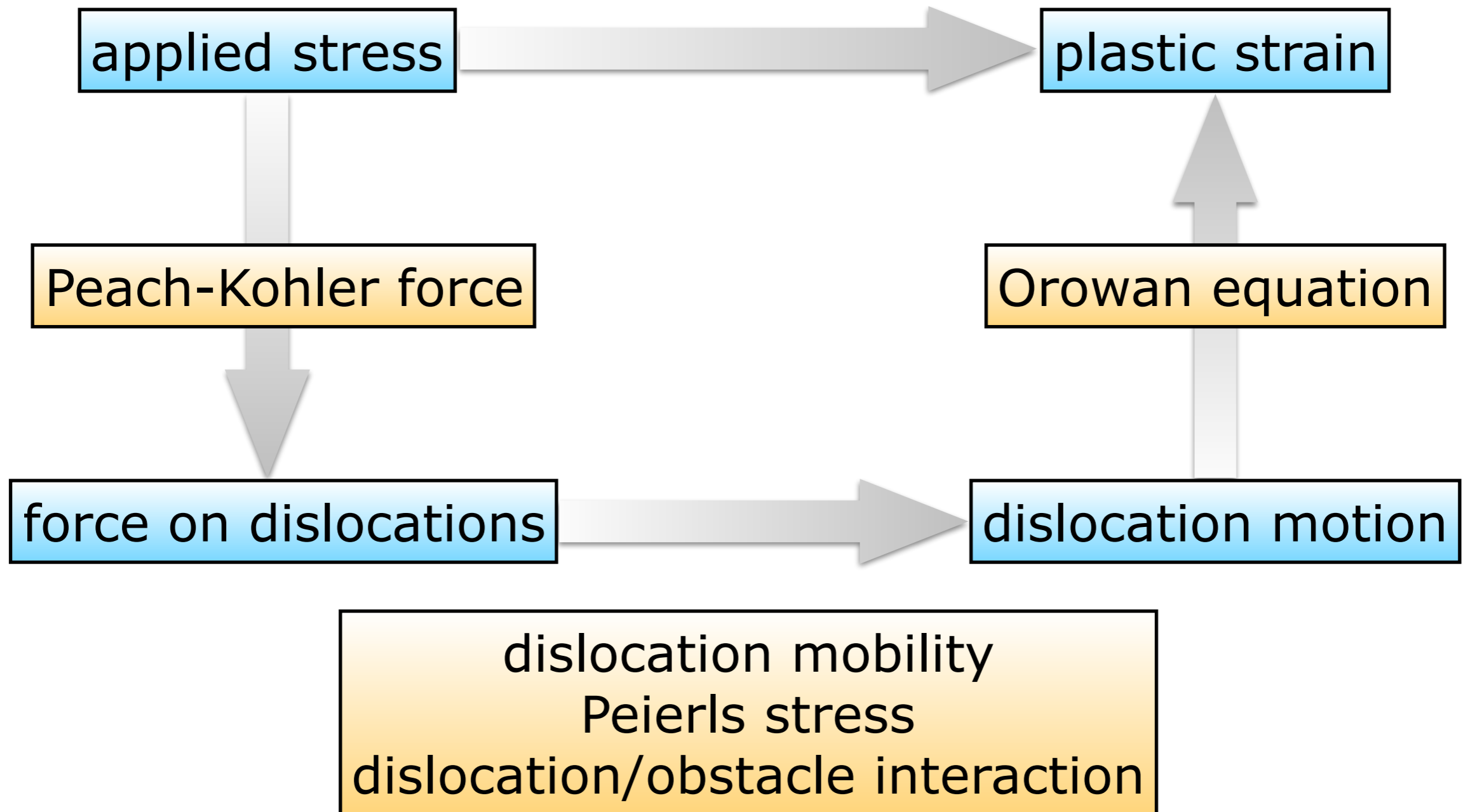


Dislocations and plastic deformation

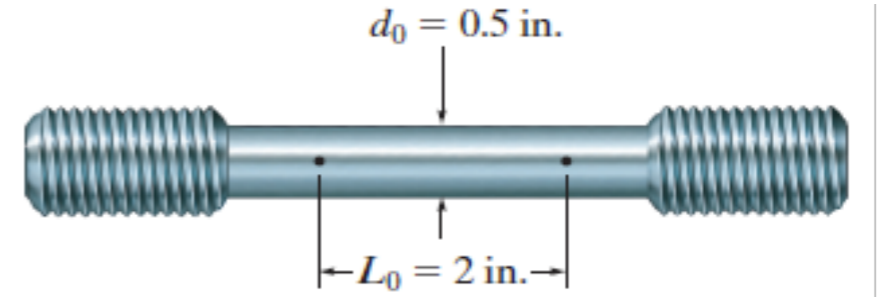


Plastic response

- Stress-strain test
- Necking, work-hardening, true stress/strain
- Multiaxial loading
- Crystal model of slip

Stress-strain diagram

- Uniaxial tension test:
 - Stress: what we do to the material
 - Strain: how the material responds
- Quantify:
 - Initial gauge length L_0 and area A_0 ; instantaneous length L and area A



Engineering stress

$$\sigma_E = \frac{P}{A_0}$$

True stress

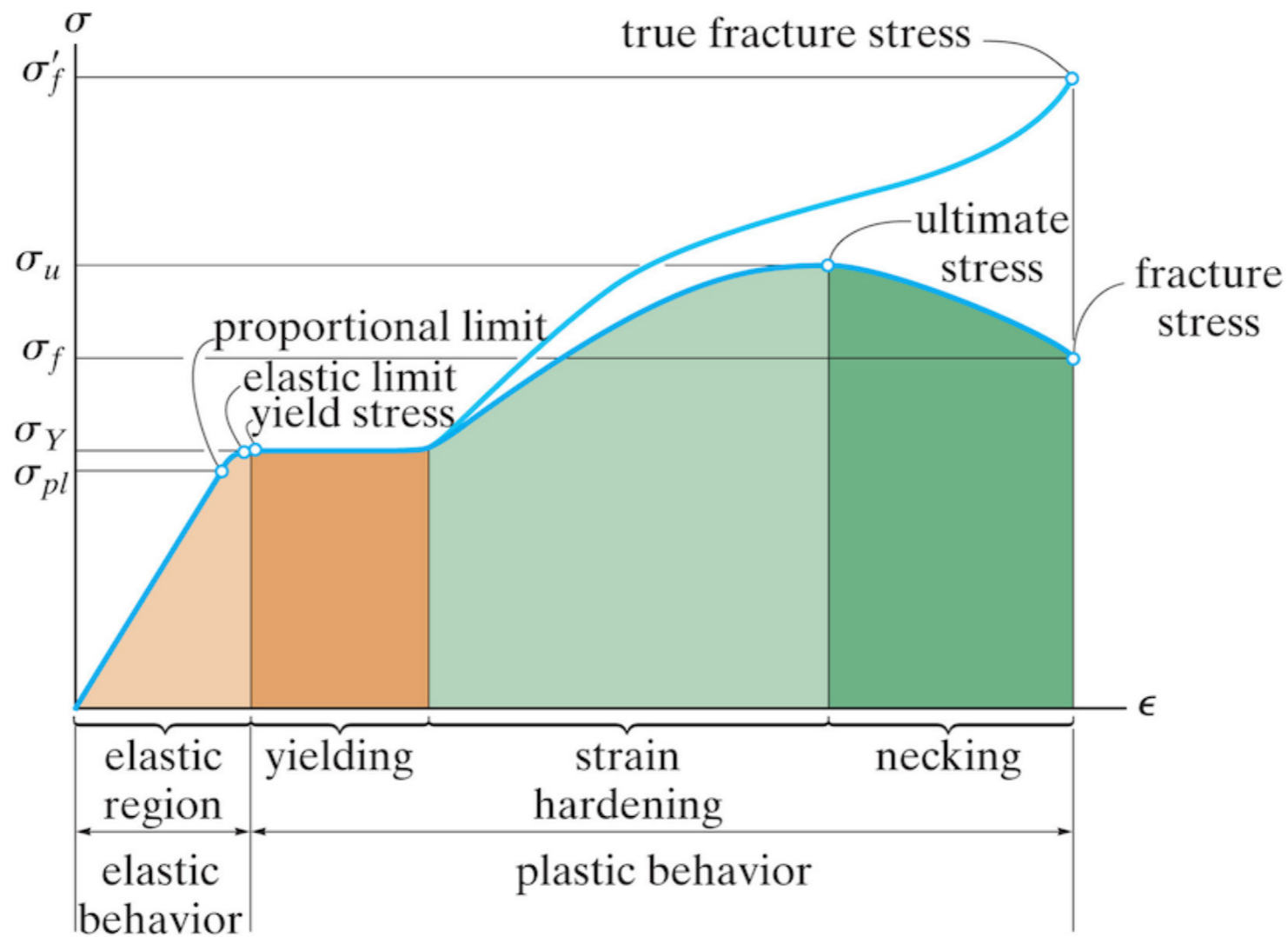
$$\sigma_T = \frac{P}{A}$$

Engineering strain

$$\epsilon_E = \frac{\delta}{L_0} = \frac{L - L_0}{L_0}$$

True strain

$$\begin{aligned} \epsilon_T &= \ln \frac{L}{L_0} = \ln \frac{A_0}{A} \\ &= \ln(1 + \epsilon_E) \end{aligned}$$



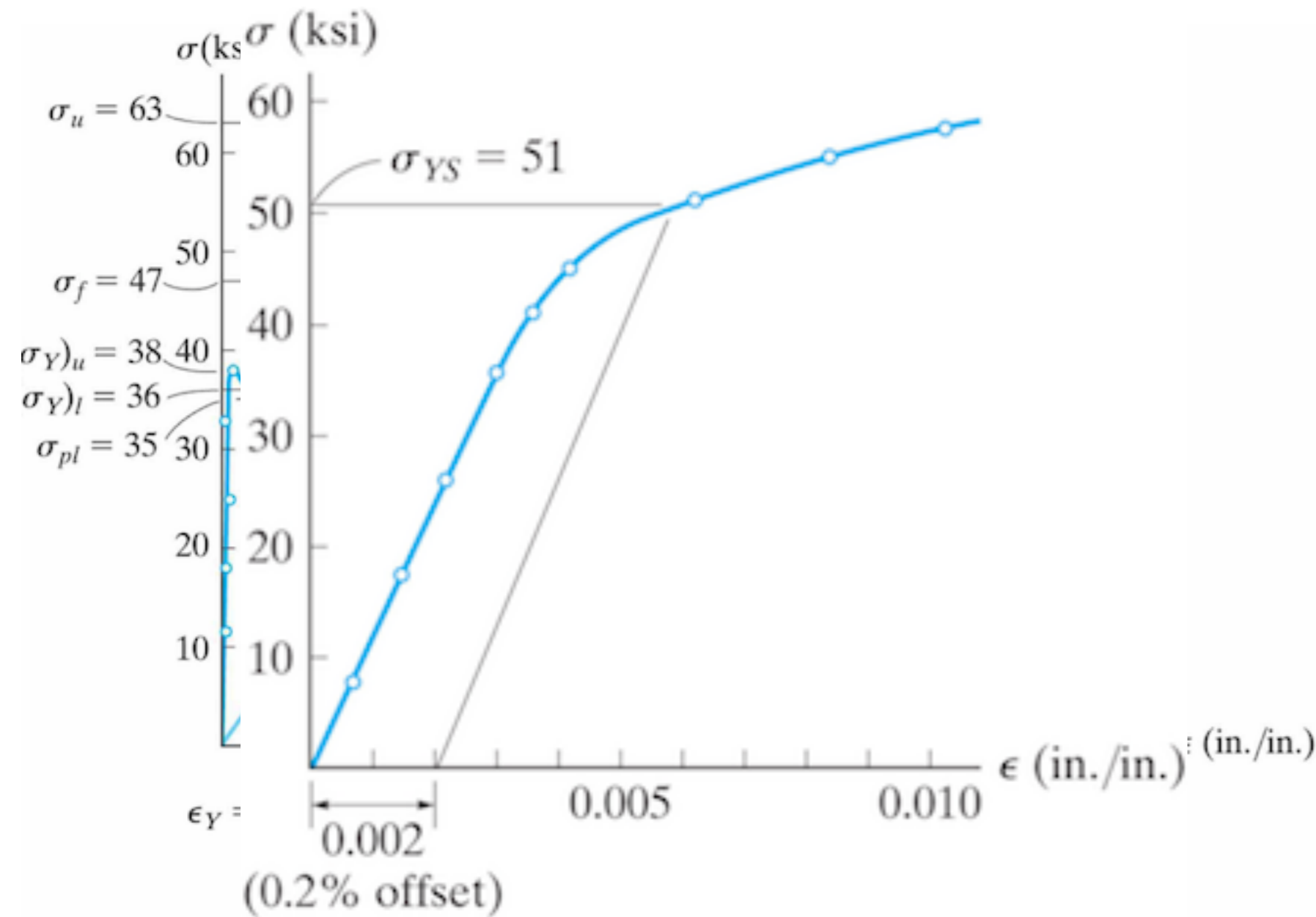
schematic steel stress-strain curve (not to scale)

Stress-strain diagram: features

- Engineering vs. true quantities
 - **Engineering:** loads and deformation from *initial geometry*
 - **True:** what the material experiences (stress), accumulated/additive dimension change (strain: 10% true + 10% true = 20% true)
- **Yield strength:** highest stress that the material can withstand without undergoing significant plastic (irreversible) deformation
 - May be defined by a **yield point** (rapid drop in stress at yield)
 - May be defined as 0.2% offset (stress to get 0.2% plastic strain)
- **Ultimate strength:** is the maximum value of stress (engineering stress) that the material can withstand
- **Fracture stress:** the value of stress at fracture
- **Stiffness:** ratio of stress to strain, primarily of interest in the elastic region. (elastic moduli)
- **Ductility:** Materials that undergo large strain before fracture are classified as ductile materials. Necks before failure
- Percent elongation: $100(L_f - L_0)/L_0$
- Percent reduction in area: $100(A_0 - A_f)/A_0$

Stress-strain diagram: ductile materials

- Rupture occurs along a cone-shaped surface that forms an angle of approximately 45° with the original surface of the specimen ("cup-cone" shape)



Shear is primarily responsible for failure in ductile materials

Axial loading: maximum shear stress occurs at 45°

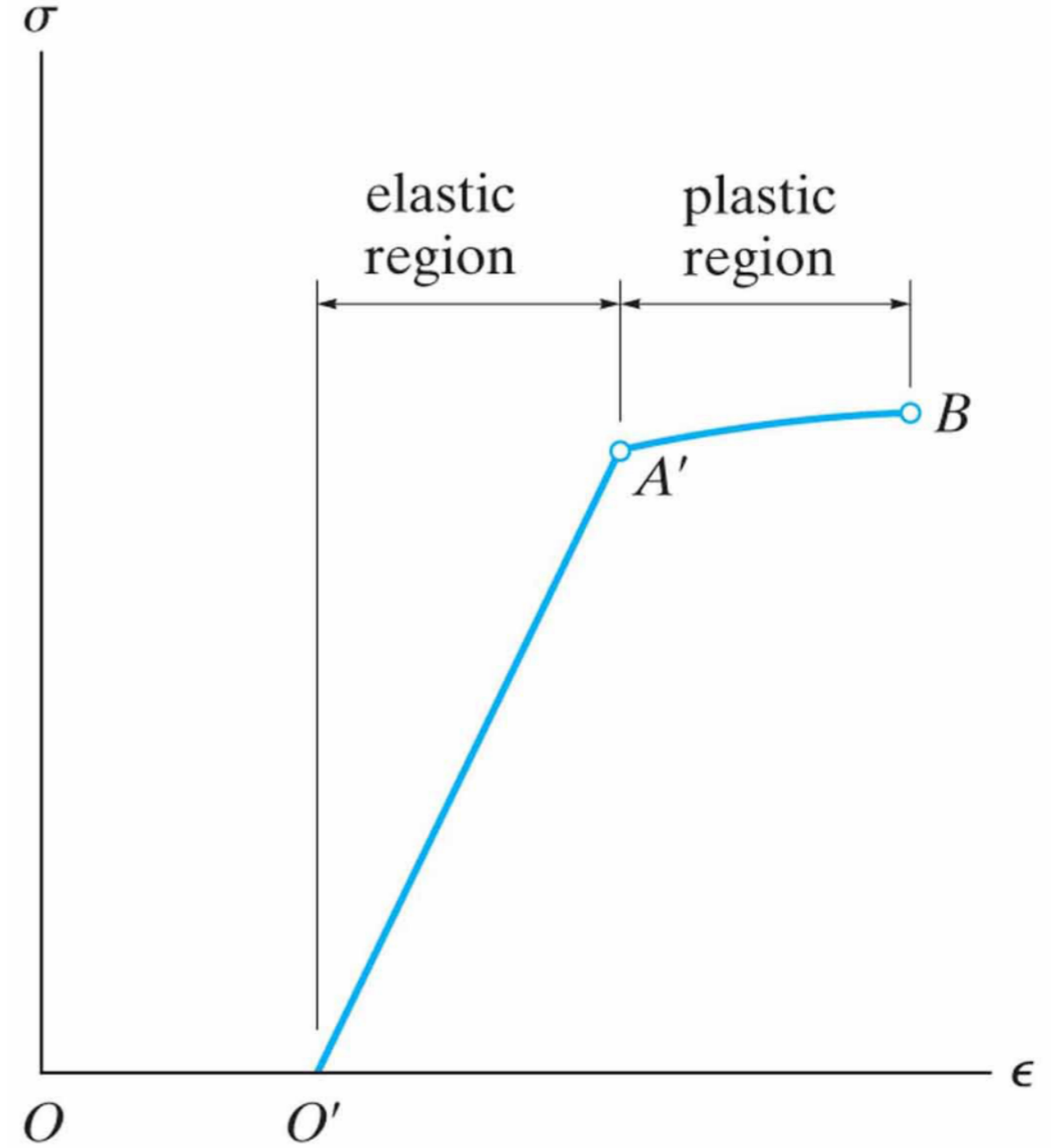
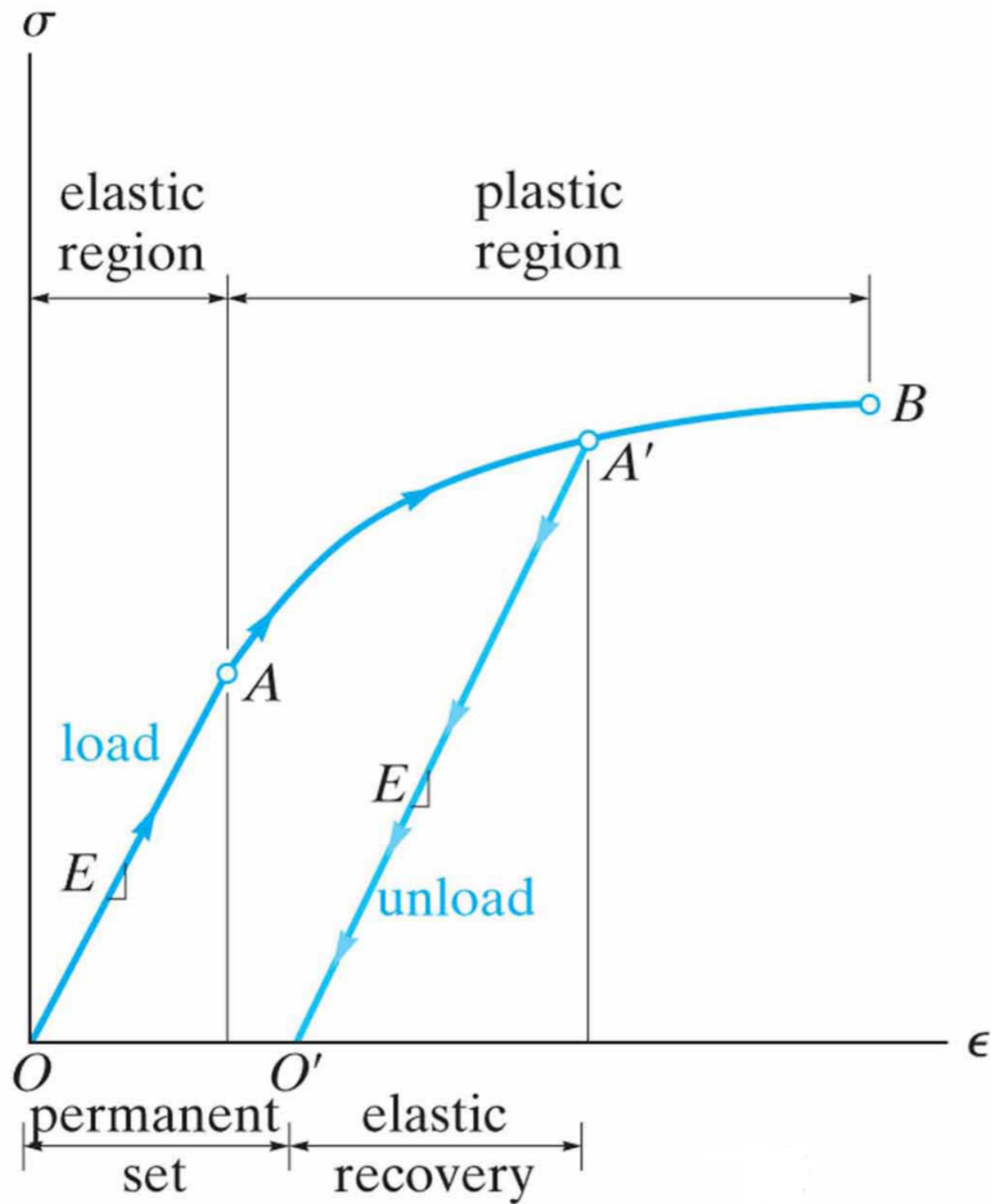


Necking

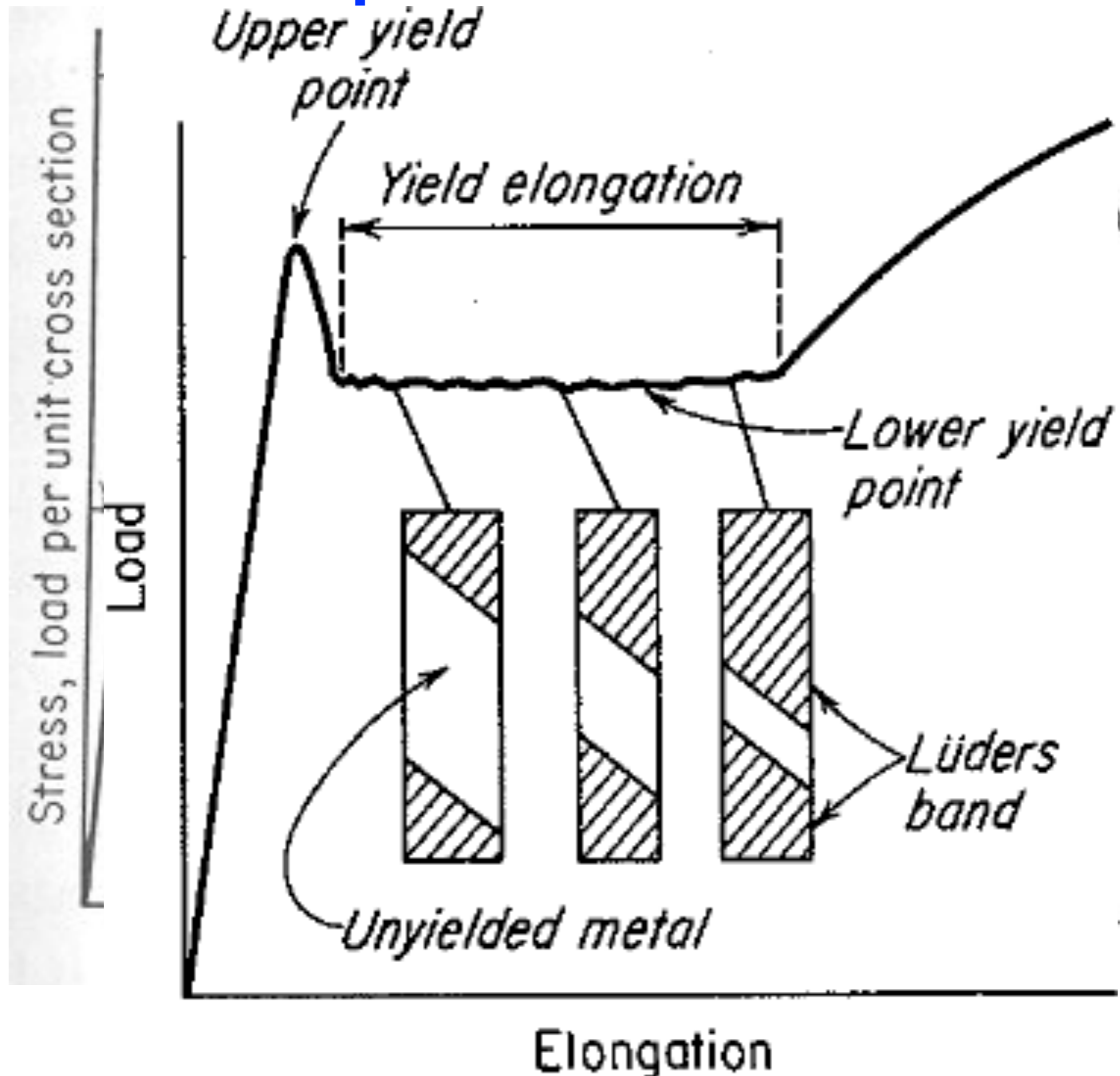


Rupture

Strain hardening



Yield point and Lüders band



From uniaxial to multiaxial stress

σ_i = principal stresses

Rankine: maximum principal stress $>$ Y_S

$$\max\{|\sigma_1|, |\sigma_2|, |\sigma_3|\} > \sigma_{Y_S}$$

Tresca: maximum shear stress $>$ $Y_S/2$

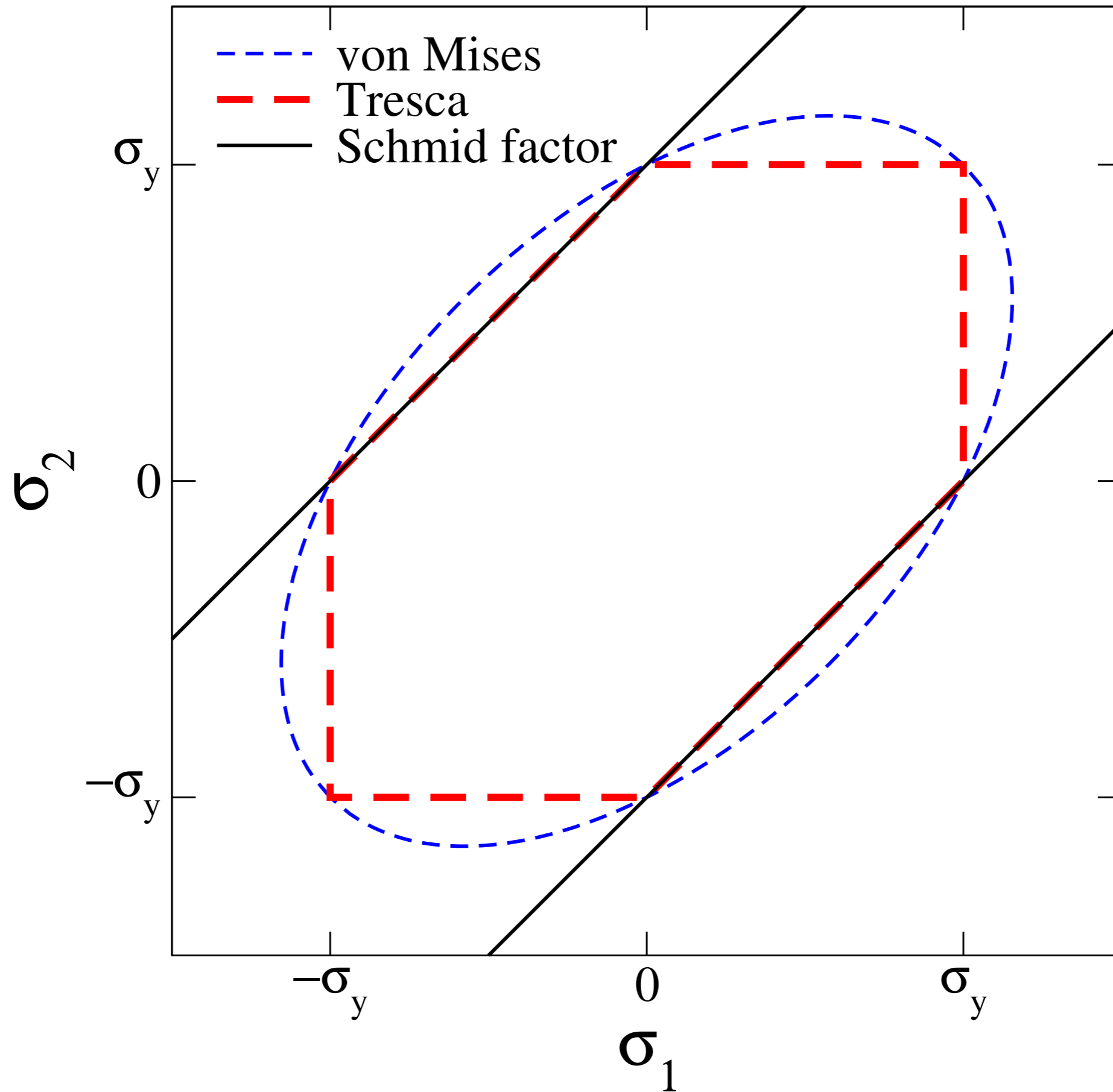
$$\max\{|\sigma_1 - \sigma_2|, |\sigma_2 - \sigma_3|, |\sigma_3 - \sigma_1|\} > \sigma_{Y_S}$$

von Mises: maximum distortion energy $>$ yield

$$(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 > 2\sigma_{Y_S}^2$$

$$\begin{aligned} (\sigma_{xx} - \sigma_{yy})^2 + (\sigma_{yy} - \sigma_{zz})^2 + (\sigma_{zz} - \sigma_{xx})^2 \\ + 6(\sigma_{xy}^2 + \sigma_{yz}^2 + \sigma_{zx}^2) > 2\sigma_{Y_S}^2 \end{aligned}$$

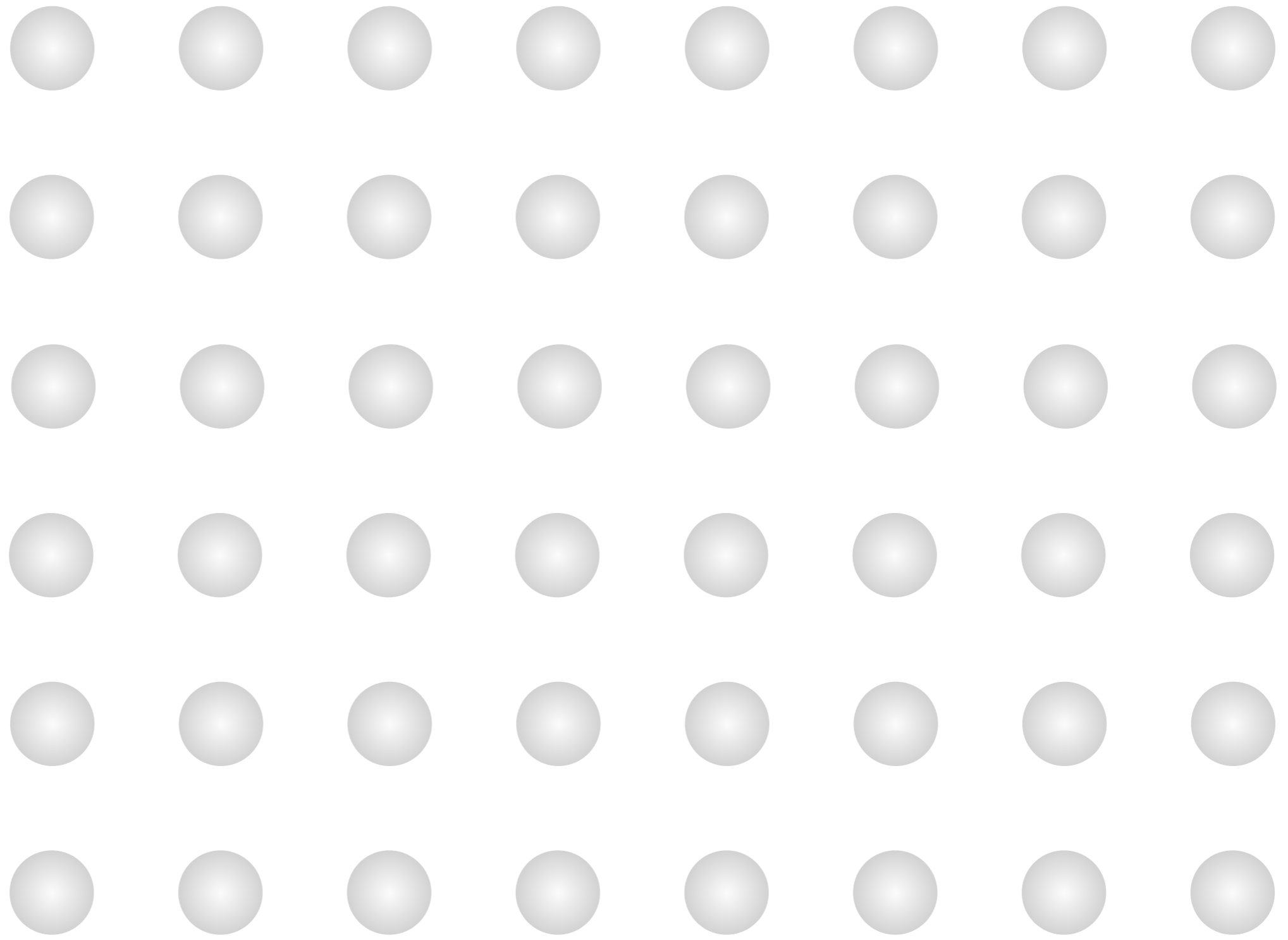
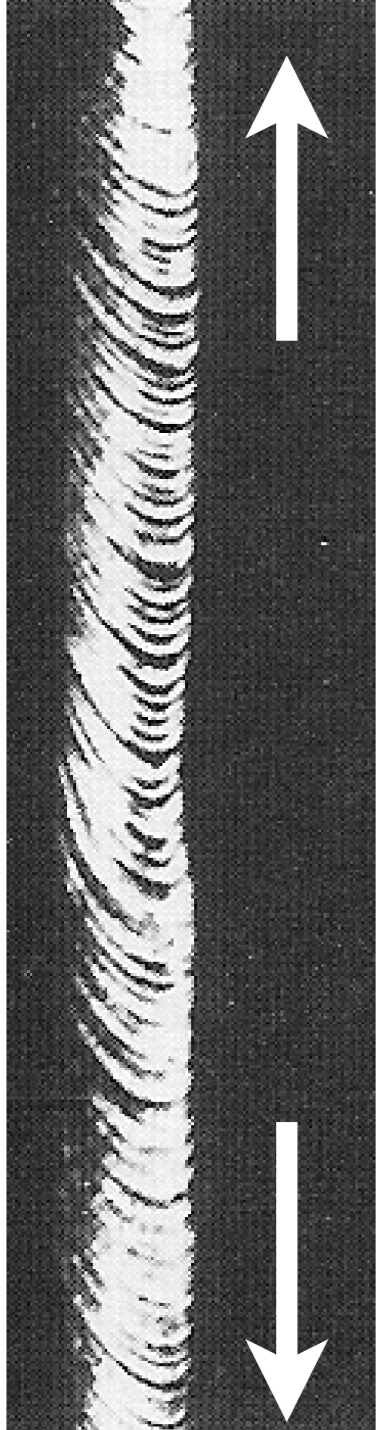
Biaxial stress: yield surface



Basic theory of plastic deformation: slip

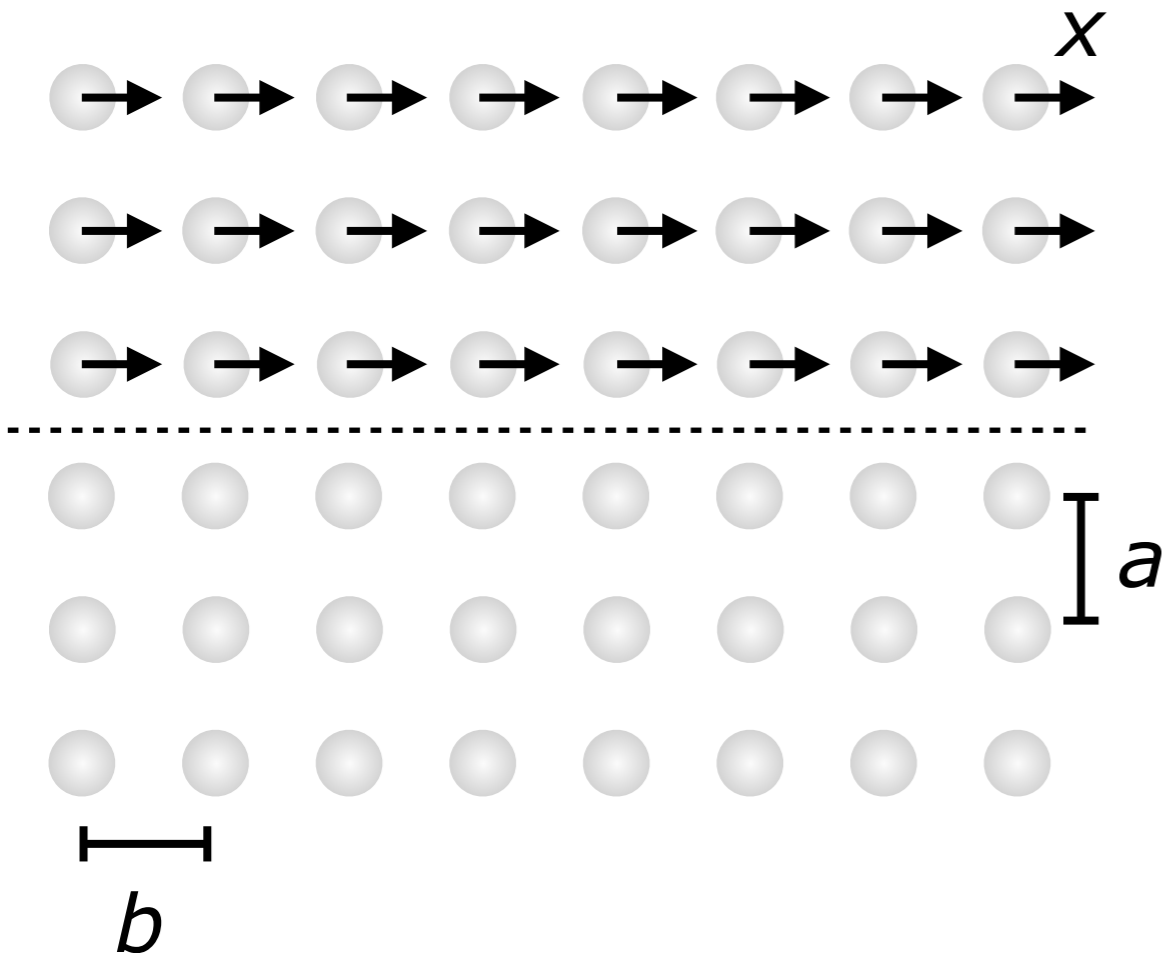
- Plastic deformation involves **flow** (no volume change) due to **shear**
- Suggests **slip** of crystal planes past each other.

single crystal
hcp Zn



Basic theory of plastic deformation: slip

- Plastic deformation involves **flow** (no volume change) due to **shear**
- Suggests **slip** of crystal planes past each other.



$$E_{\text{surface}} = \frac{\text{(energy of surface)}}{\text{(area of surface)}} \approx \left(\text{prefactor}\right) \left[1 - \cos\left(2\pi\frac{x}{b}\right)\right]$$

$$\tau = \frac{dE_{\text{surface}}}{dx} = \left(\text{prefactor}\right) \frac{2\pi}{b} \sin\left(2\pi\frac{x}{b}\right)$$

$$\tau \approx \left(\text{prefactor}\right) \left(\frac{2\pi}{b}\right)^2 x$$

$$= \left(\text{prefactor}\right) \left(\frac{2\pi}{b}\right)^2 a \frac{x}{a}$$

$$= G\gamma$$

$$E_{\text{surface}} = \frac{Gb^2}{(2\pi)^2 a} \left(1 - \cos\left(\frac{2\pi x}{b}\right)\right) \quad \text{and} \quad \tau = \frac{Gb}{2\pi a} \sin\left(\frac{2\pi x}{b}\right)$$

Basic theory of plastic deformation: slip

- Plastic deformation involves **flow** (no volume change) due to **shear**
- Suggests **slip** of crystal planes past each other.

$$\tau_{\text{theoretical shear strength}} = \frac{Gb}{2\pi a} \approx \frac{1}{6}G \cdots \frac{1}{30}G$$

Litany of problems:

Typical metals shear strength $\sim 10^{-4} G$

Pure metal shear strength $\sim 10^{-6} G$ for fcc

No explanation of temperature or strain-rate effects

No explanation for work hardening

No explanation for alloying effects

No differentiation between brittle and ductile

Describes one system:

Metal whiskers have strengths $\sim 1\% G$

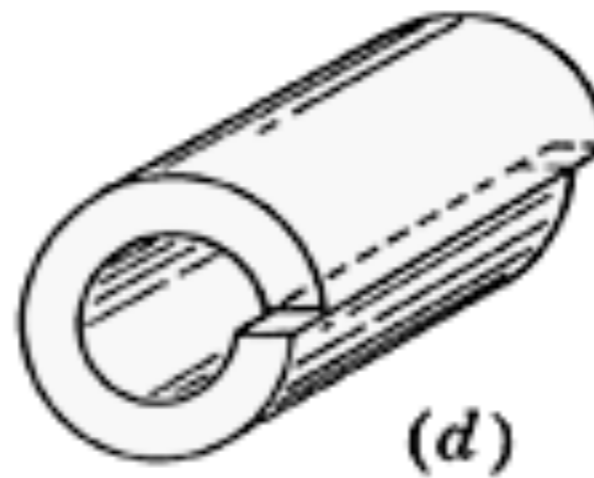
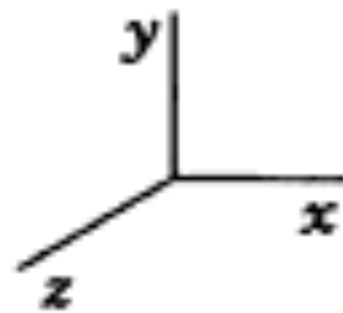
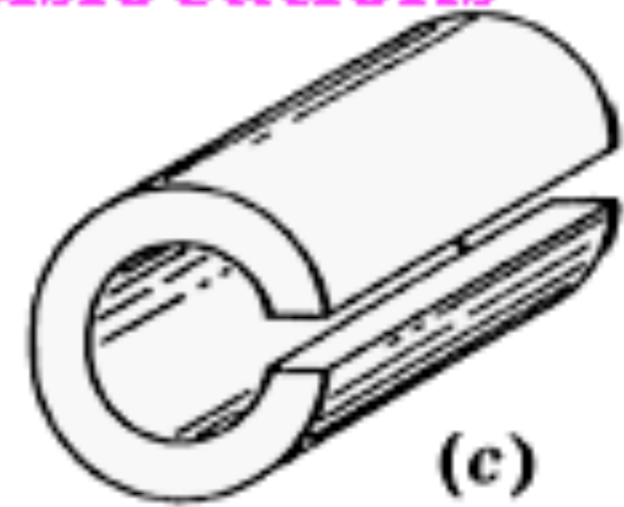
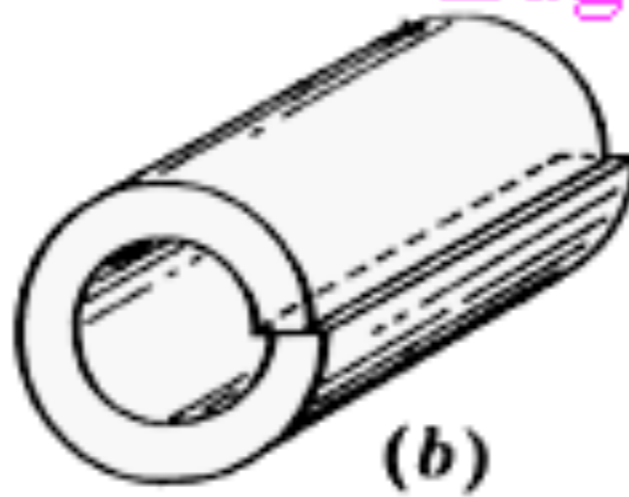
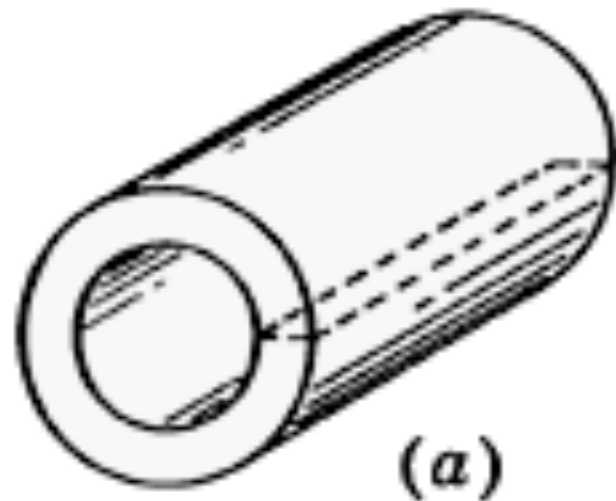
Plastic response to Dislocations

- Stress-strain test
- Necking, work-hardening, true stress/strain
- Multiaxial loading
- Crystal model of slip

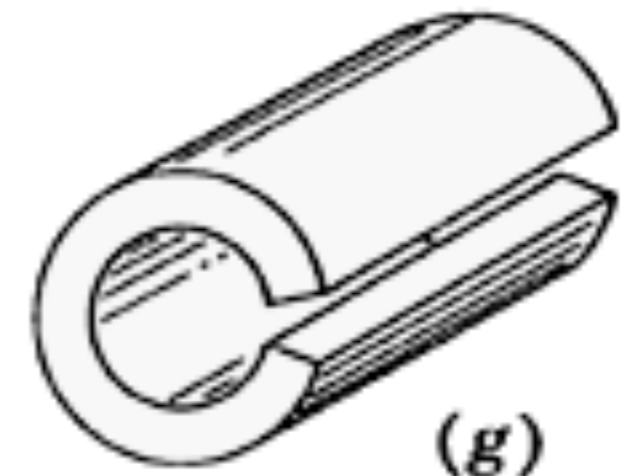
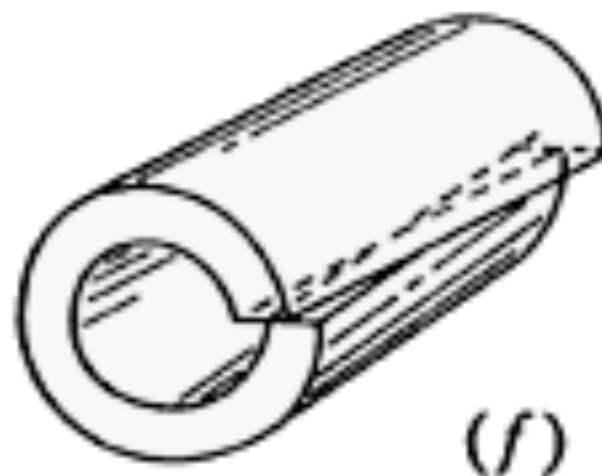
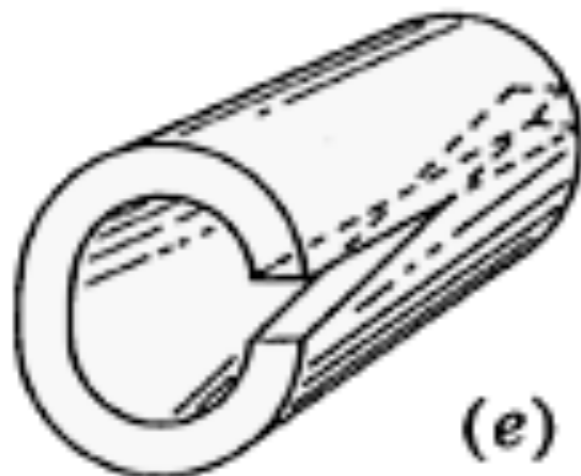
- Topological defects
- Screw, edge, mixed

Volterra tubes

Edge dislocations



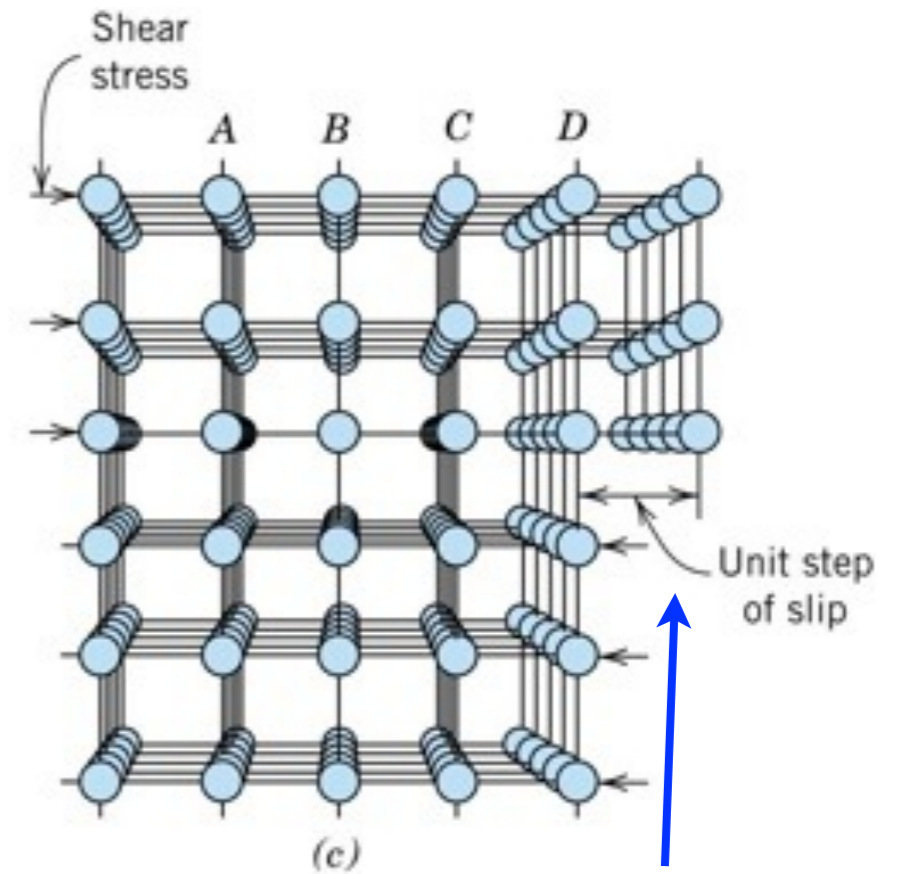
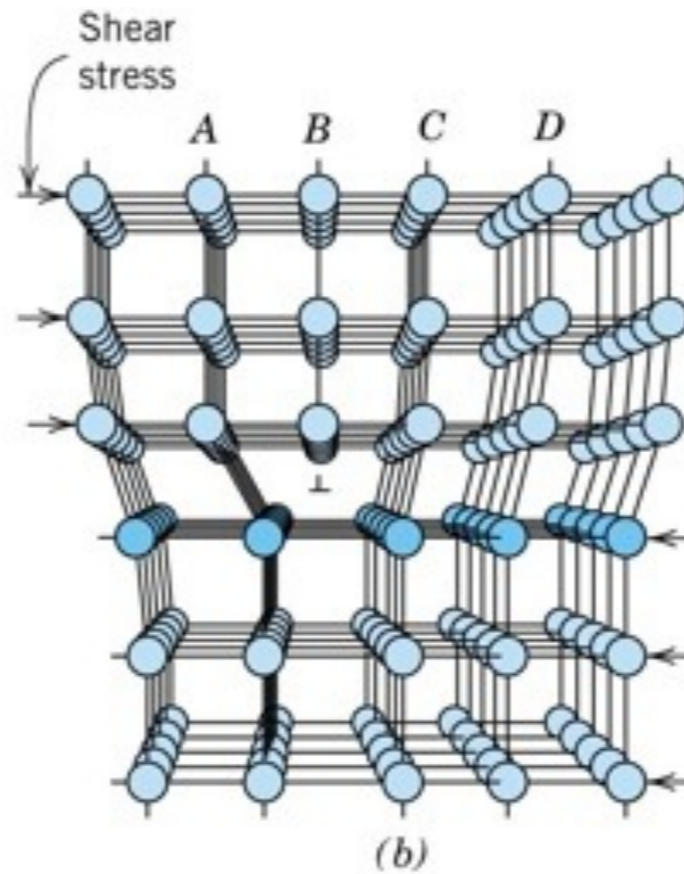
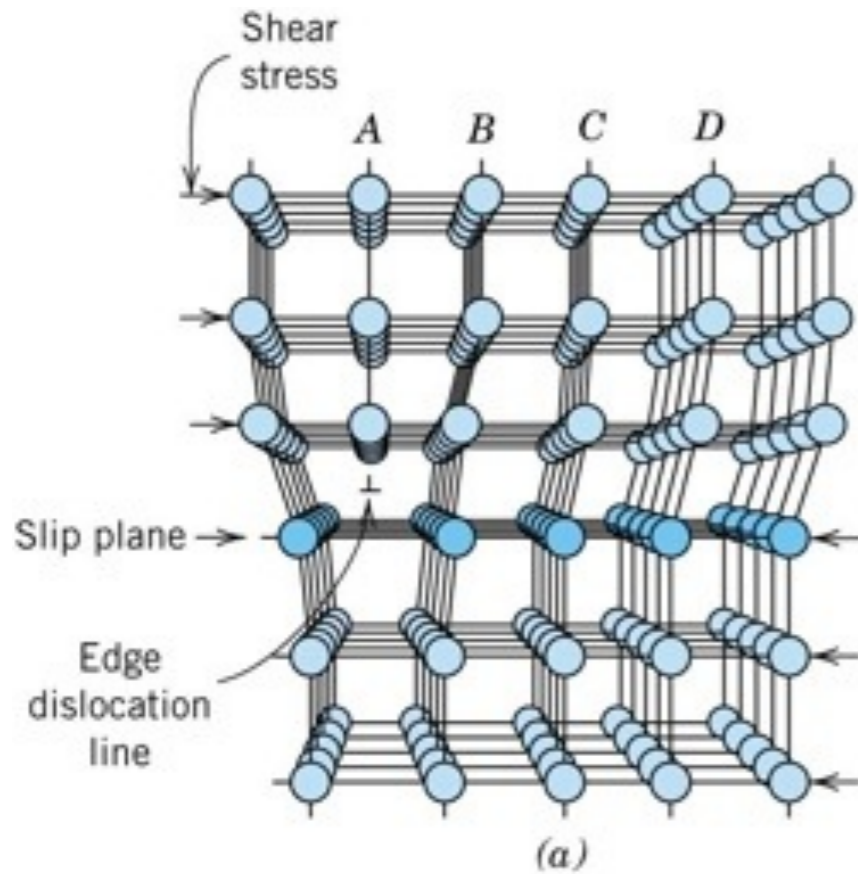
Screw dislocation



Disclinations

Dislocation plastic deformation

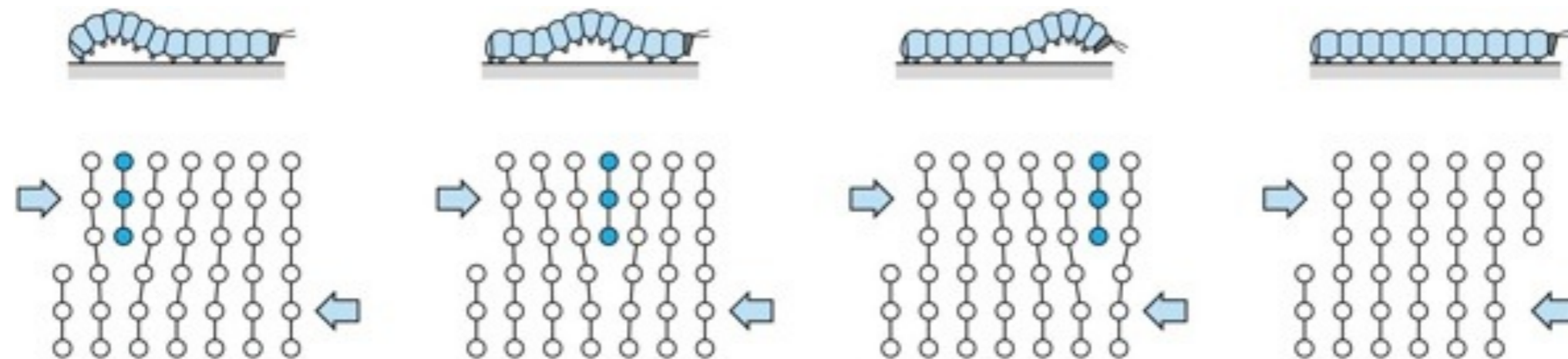
shear stress



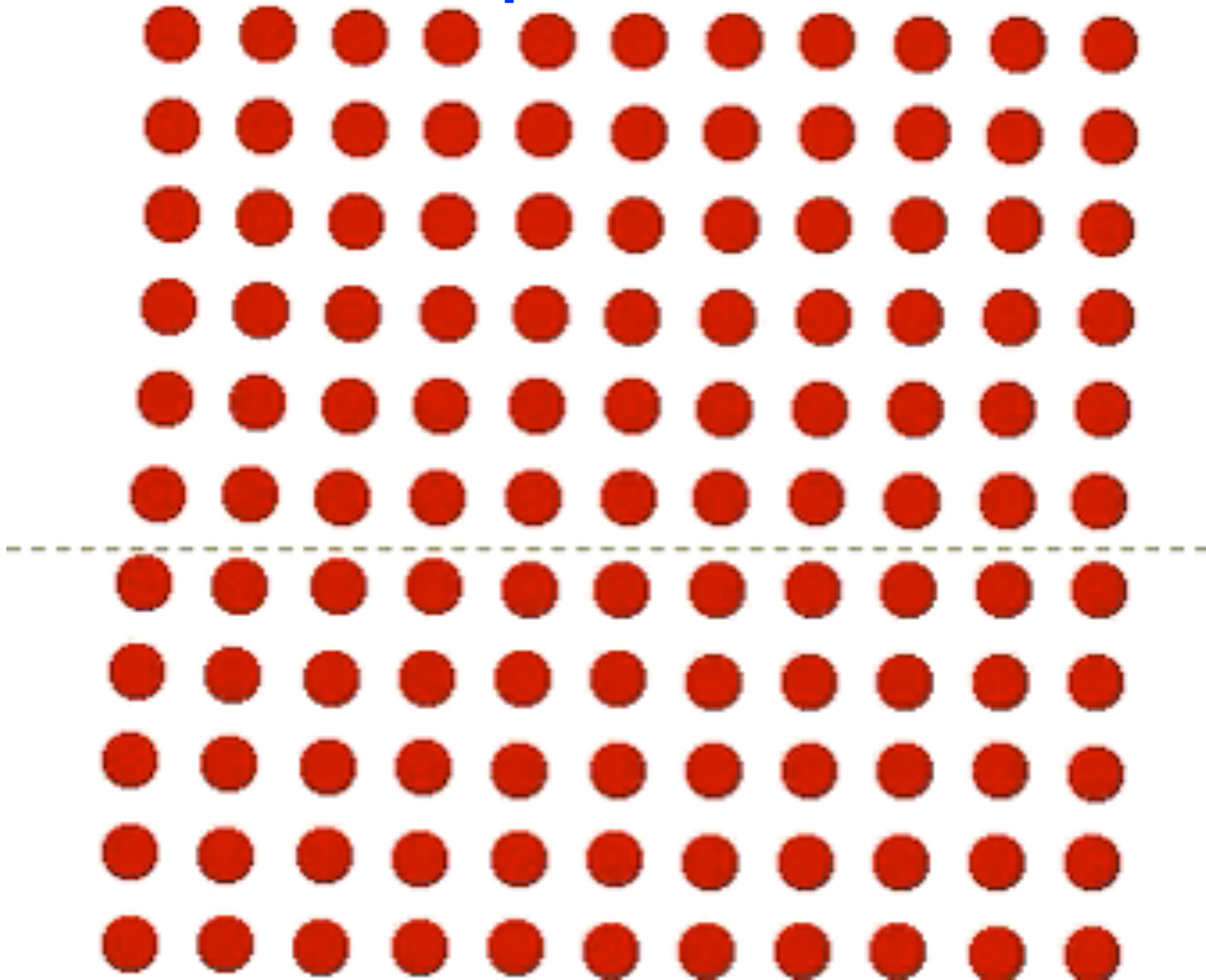
shear stress



slip by one
Burgers vector

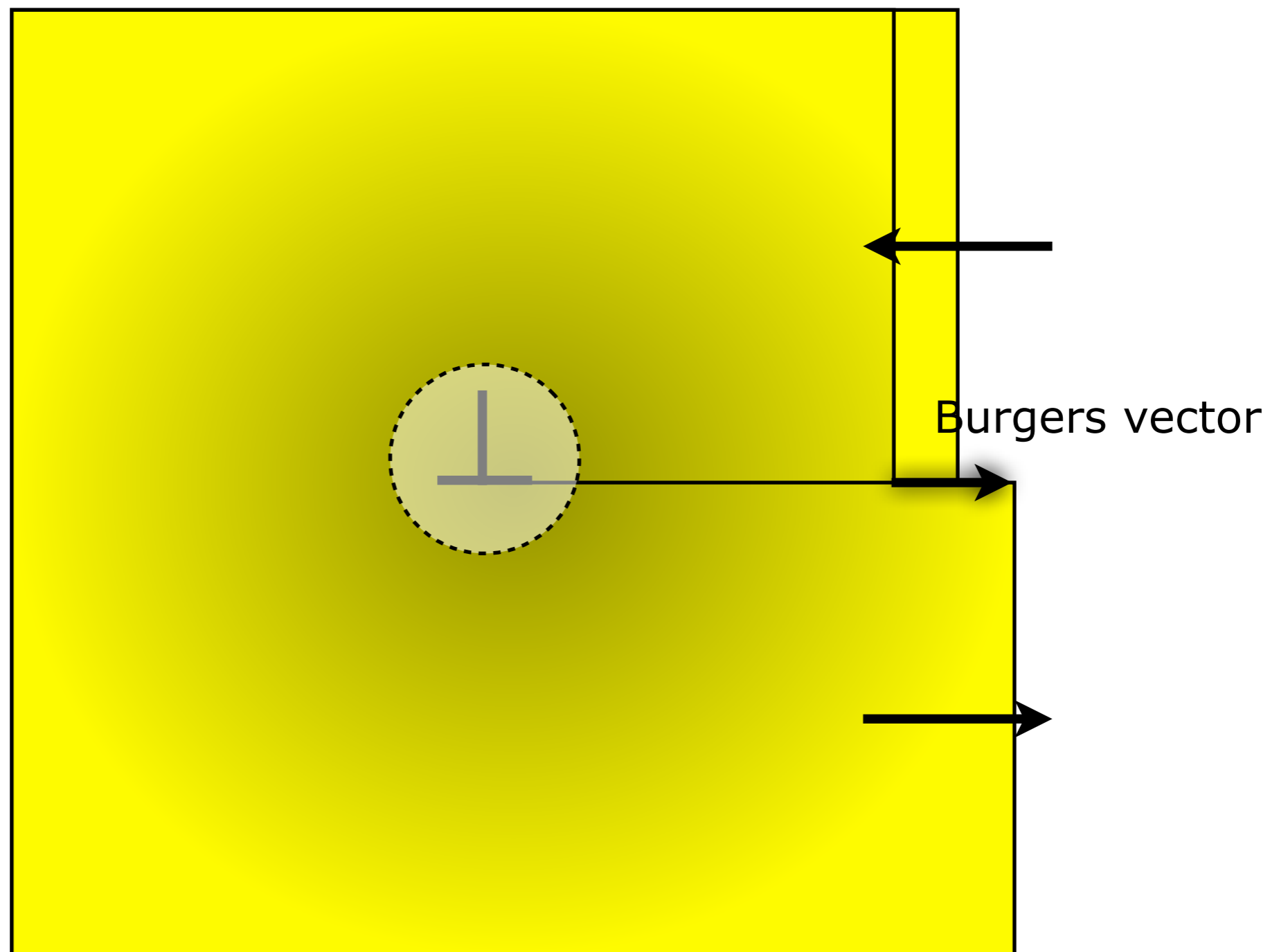


Dislocation plastic deformation



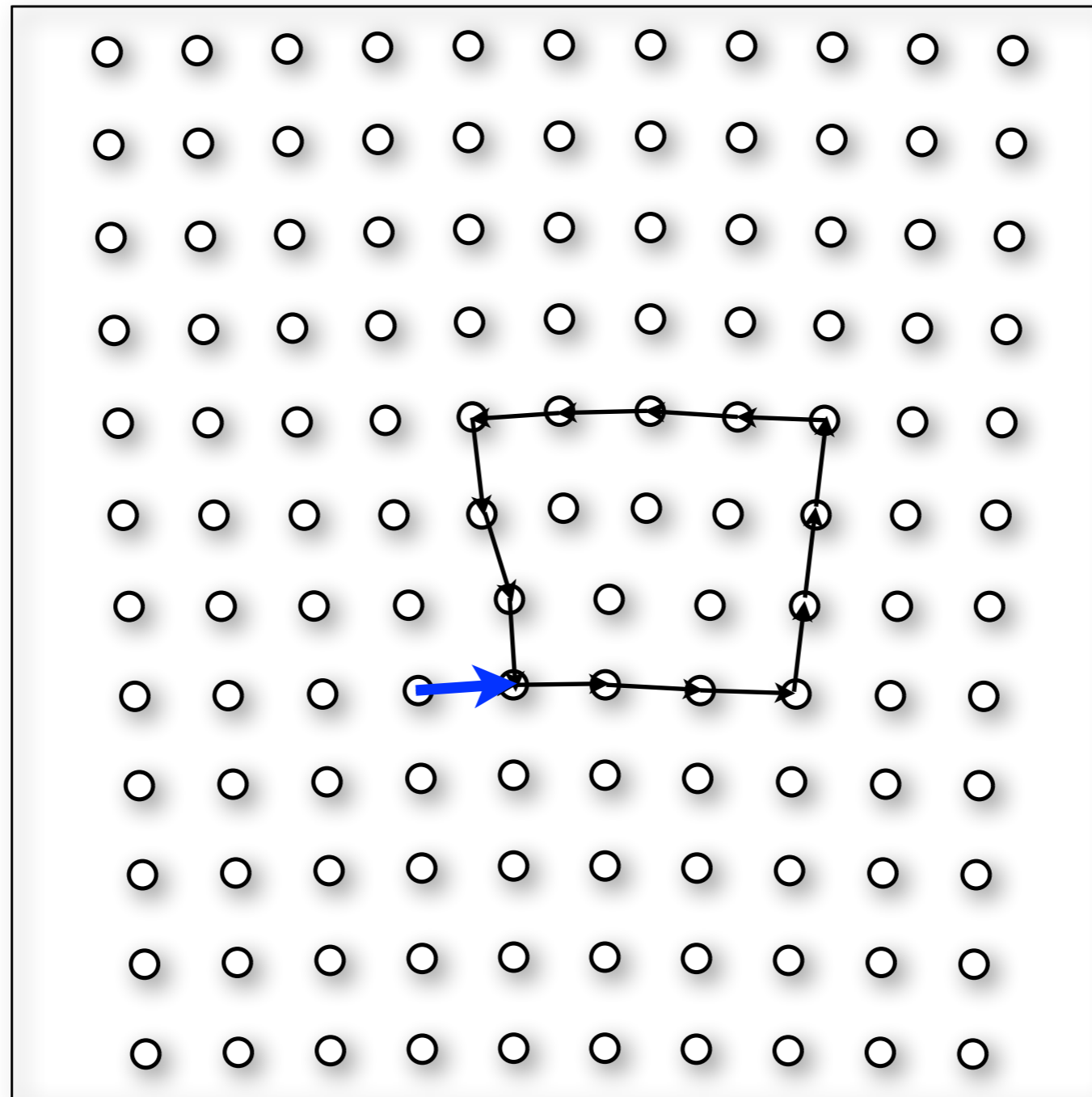
Edge dislocation

"extra" half-plane of atoms



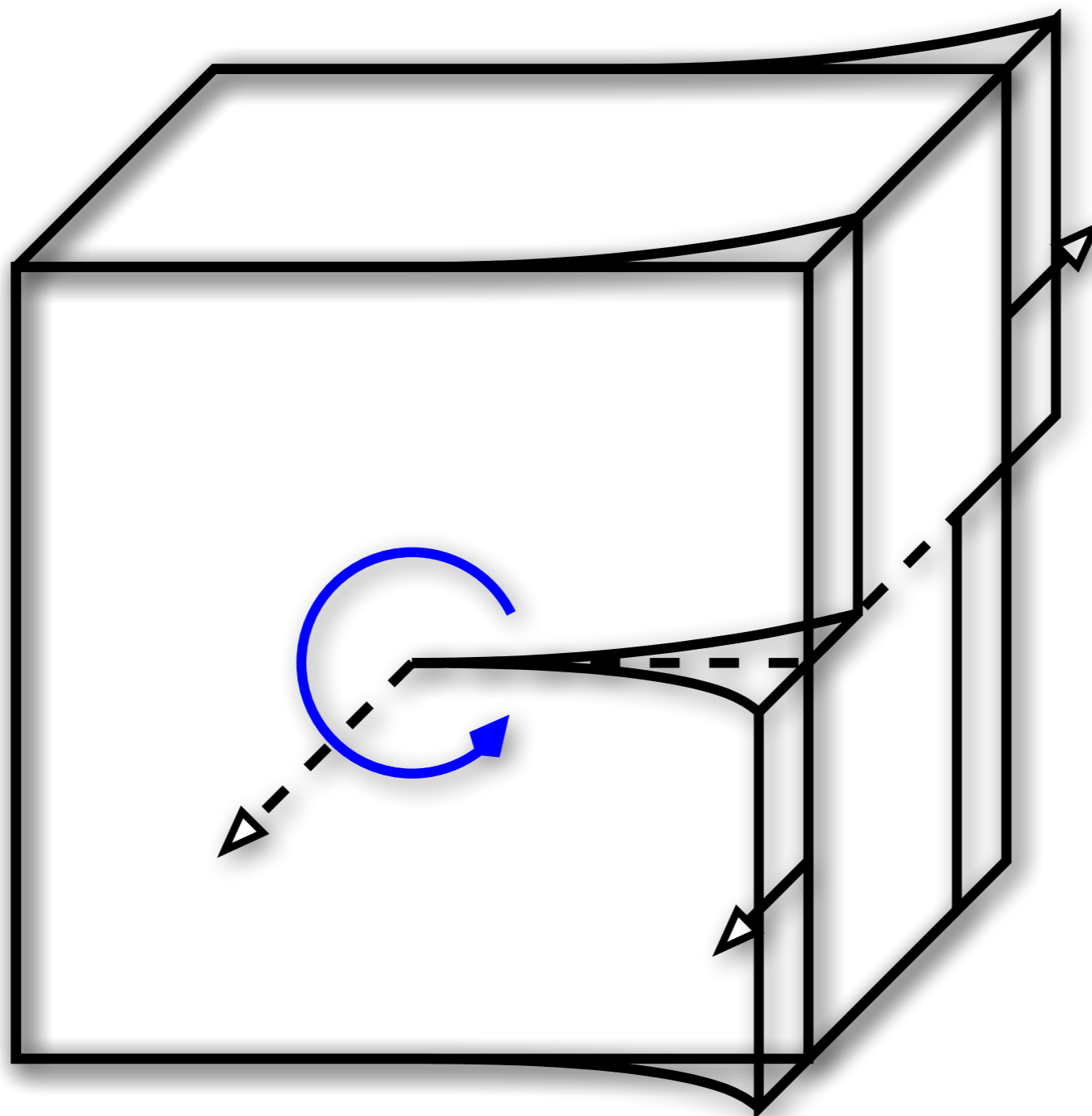
Edge dislocation: Burgers circuit

"extra" half-plane of atoms

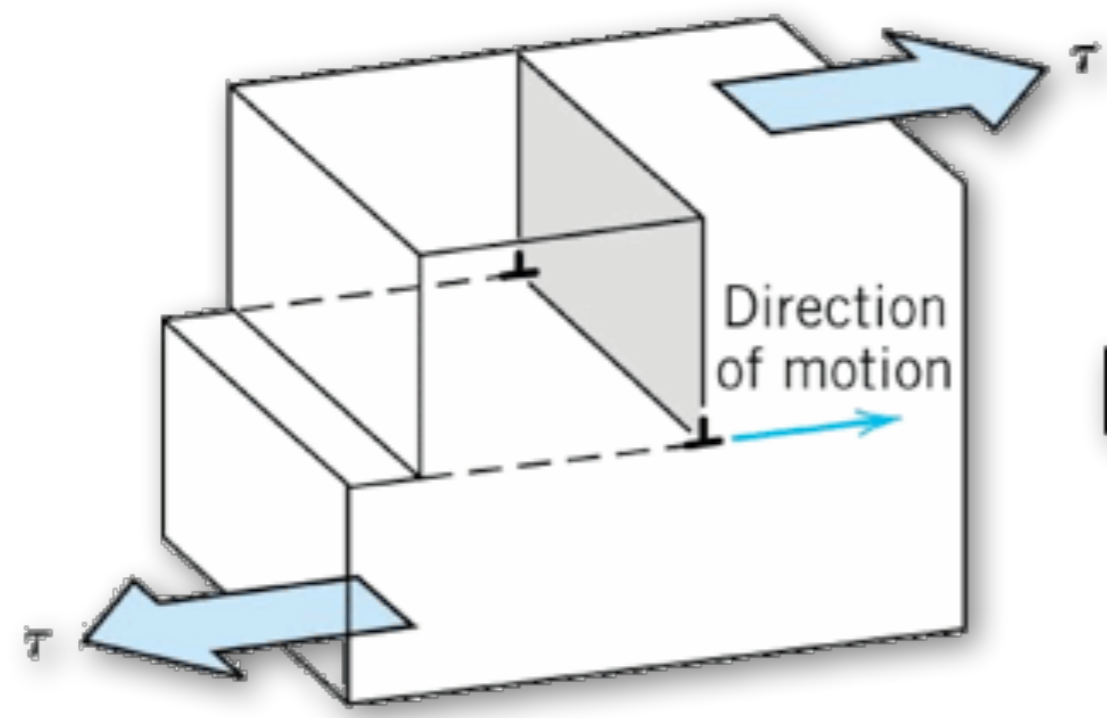


failure to close =
Burgers vector

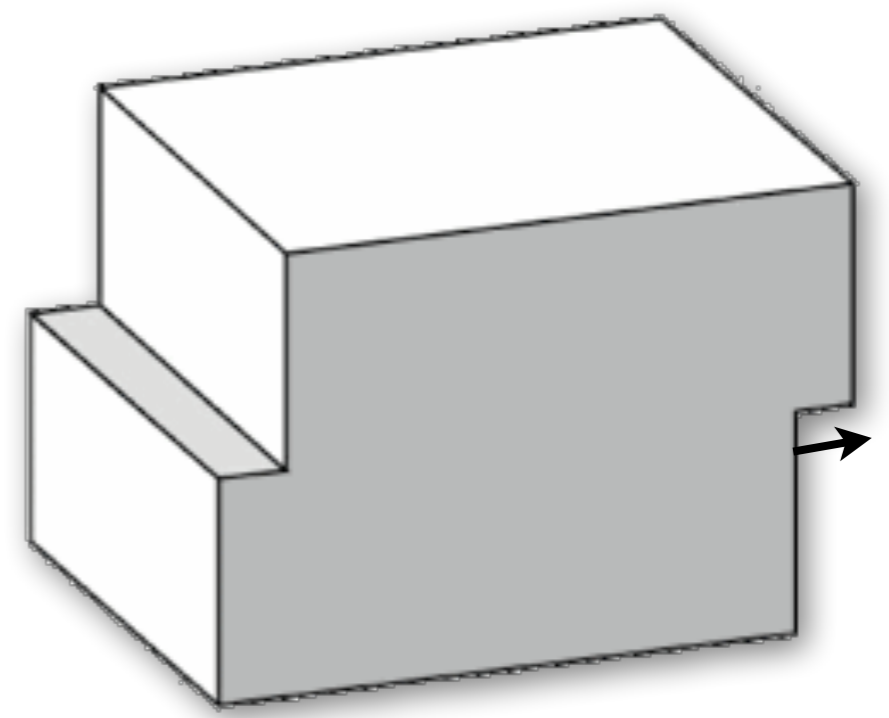
Screw dislocation



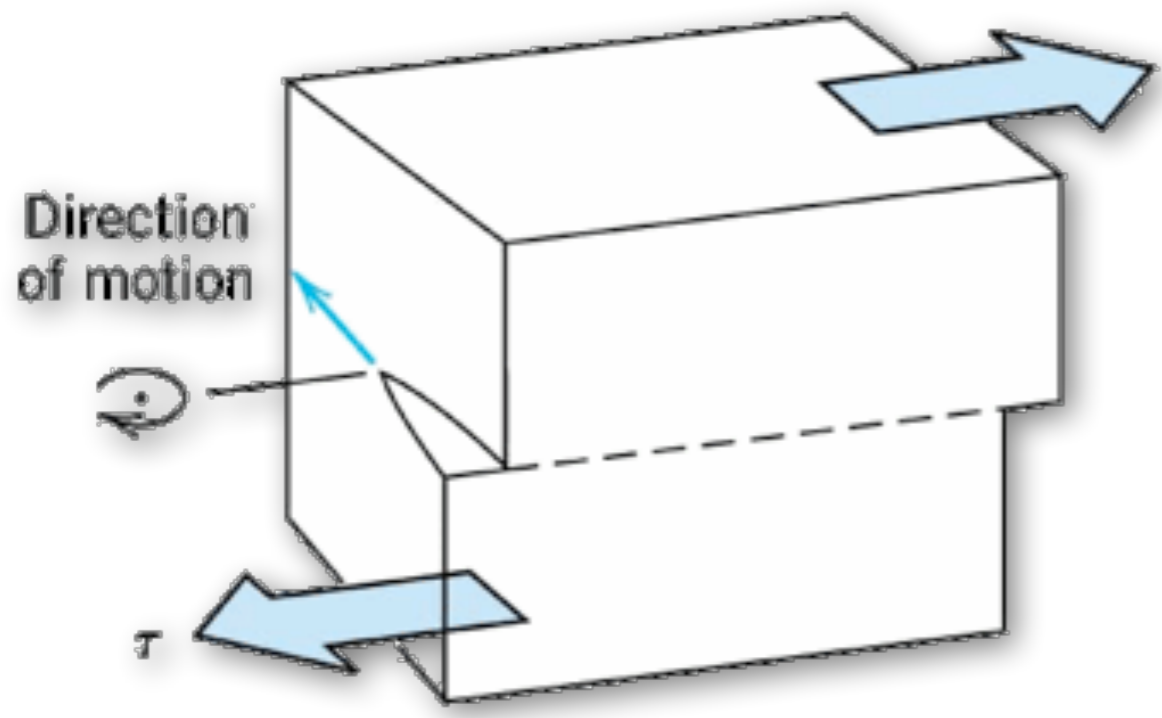
Dislocation motion: Slip steps



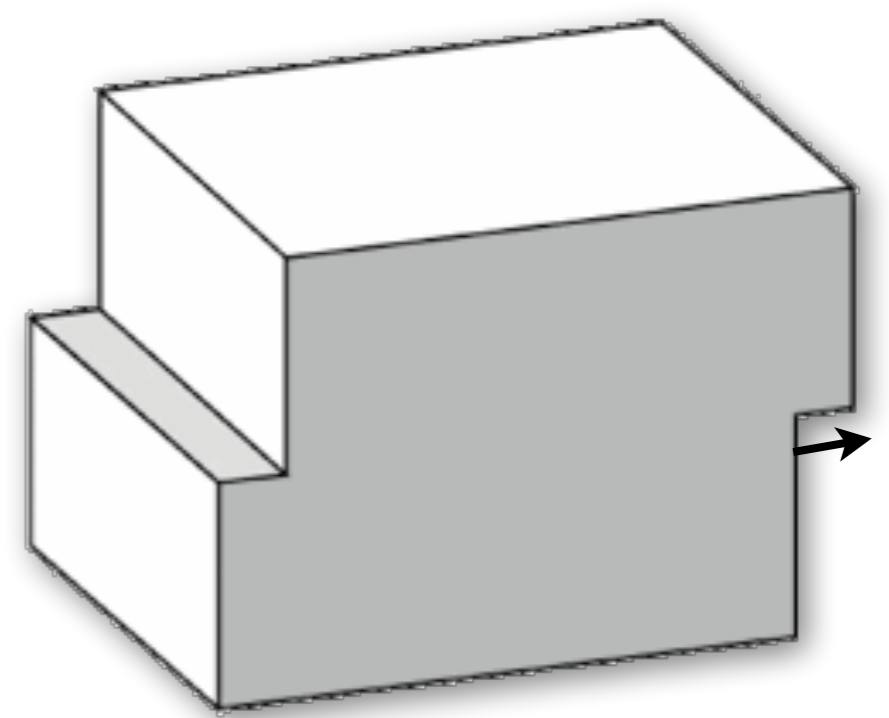
edge



same stress,
same Burgers vector,
different dislocation type,
same slip

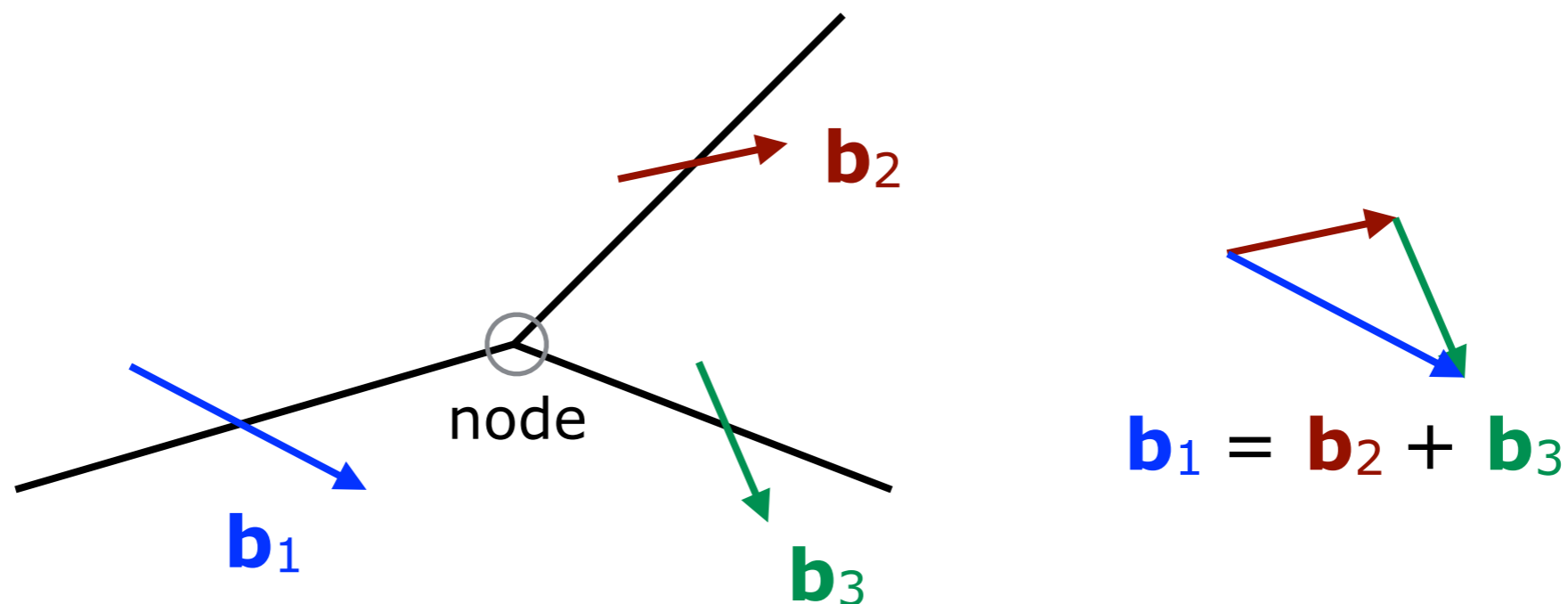


screw



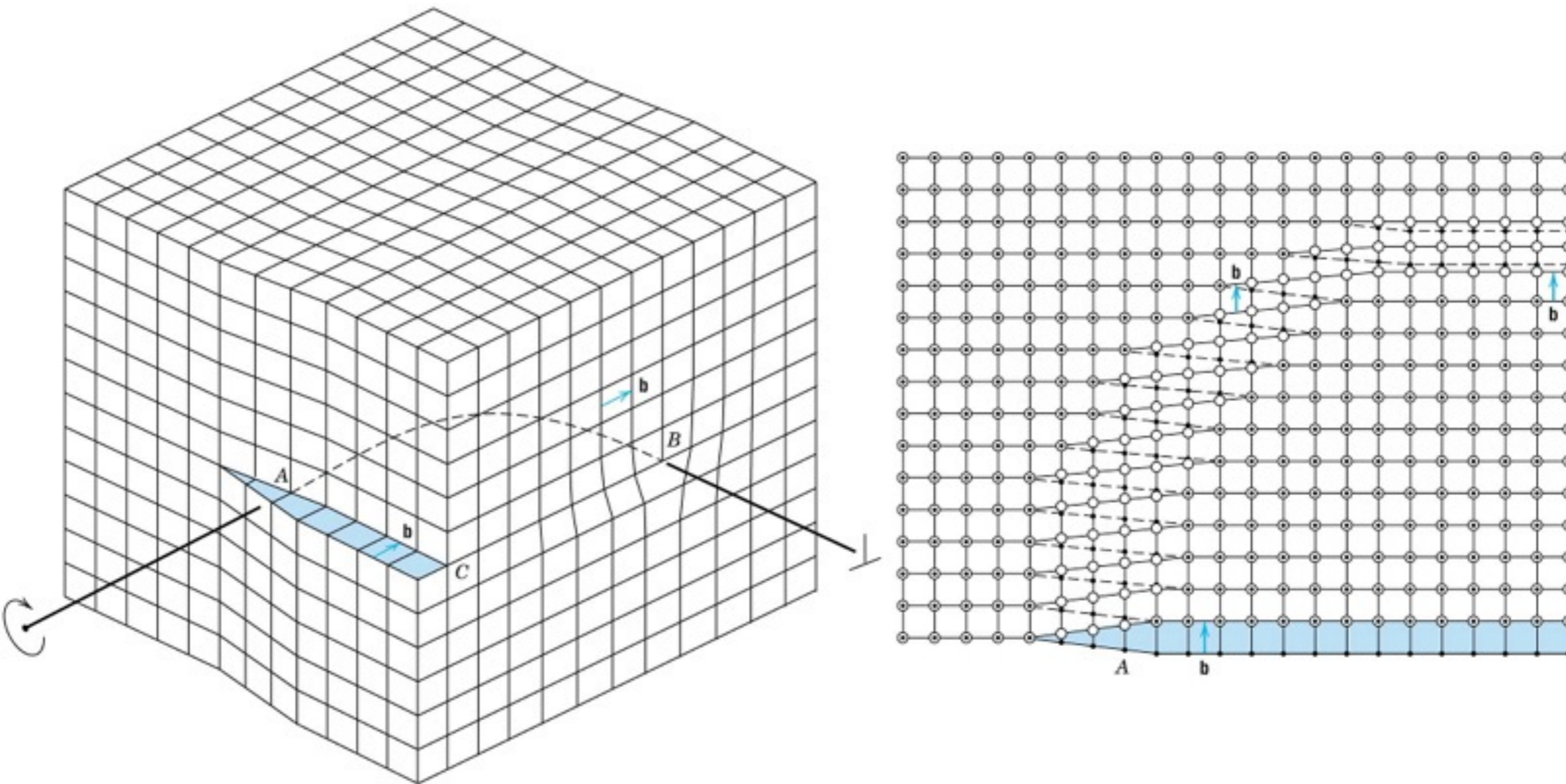
Dislocation line and Burgers vector

- Where the “Volterra cut” ends = **dislocation line** (not required to be straight!)
 - Dislocation line cannot end in the crystal: must loop, or end at a surface or interface
- Displacement after the cut = **Burgers vector** (a lattice vector, to not create planar defects (stacking fault)
 - A conserved quantity, like the “charge” of a dislocation
- Note: line direction (**t**) and Burger vector (**b**) are *paired* by the circuit

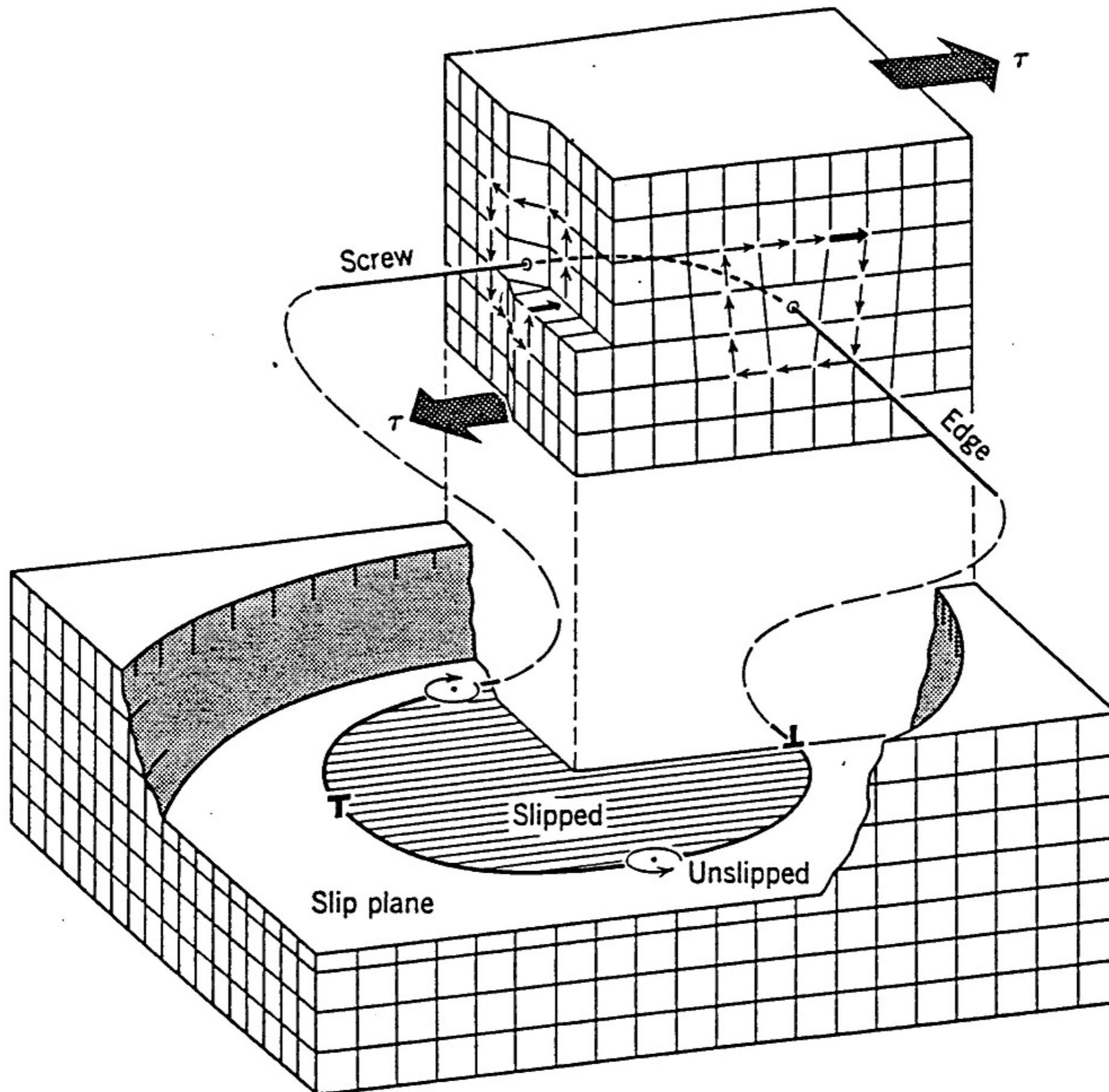


- Edge dislocation: **b** perpendicular to line direction (**t**)
- Screw dislocation: **b** parallel to line direction (**t**)
- Mixed dislocation: **b** neither perpendicular or parallel to line direction (**t**)

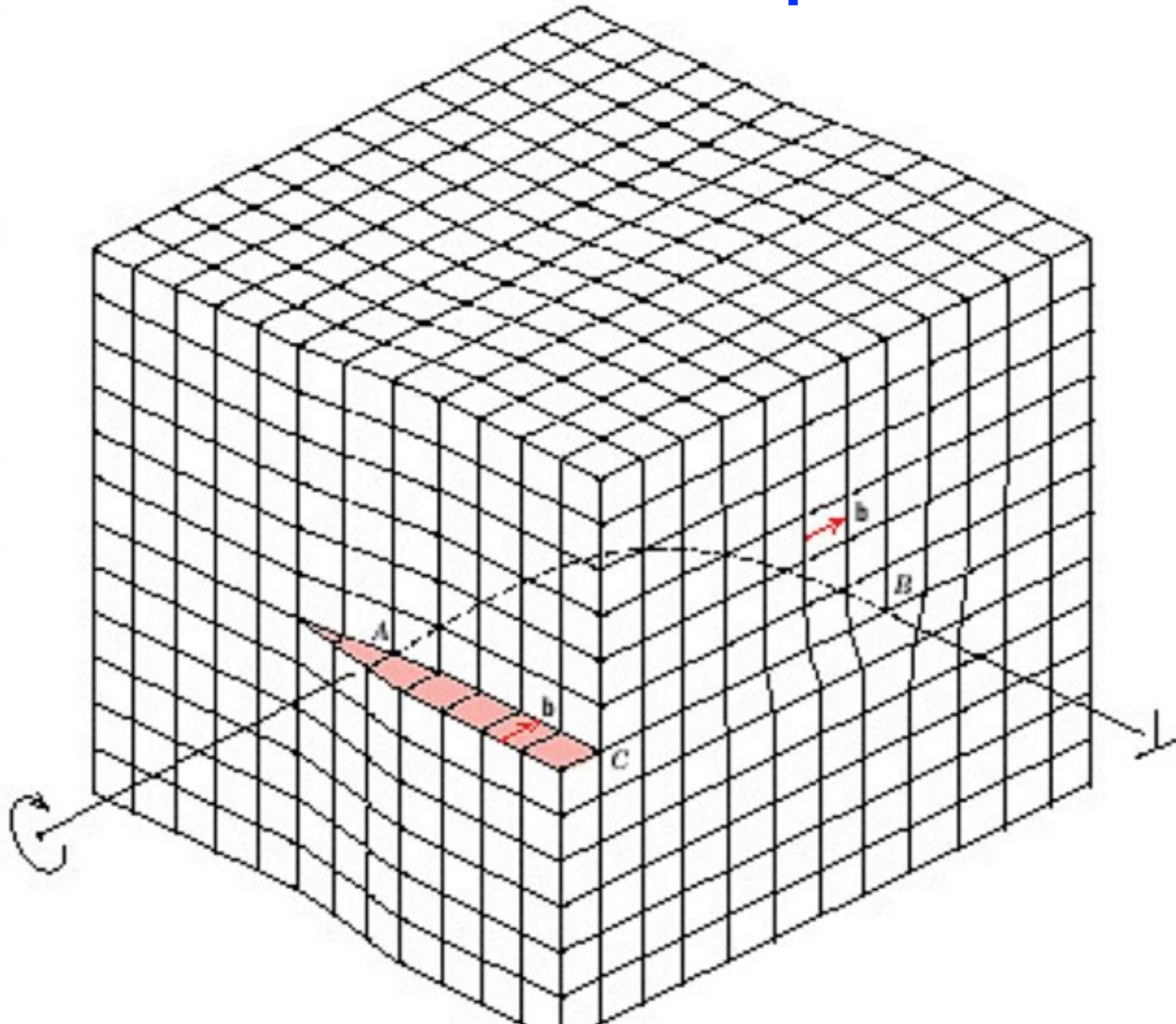
Dislocation line and Burgers vector



Dislocation loop



Dislocation loop



Dislocations types to behavior

- Topological defects
- Screw, edge, mixed

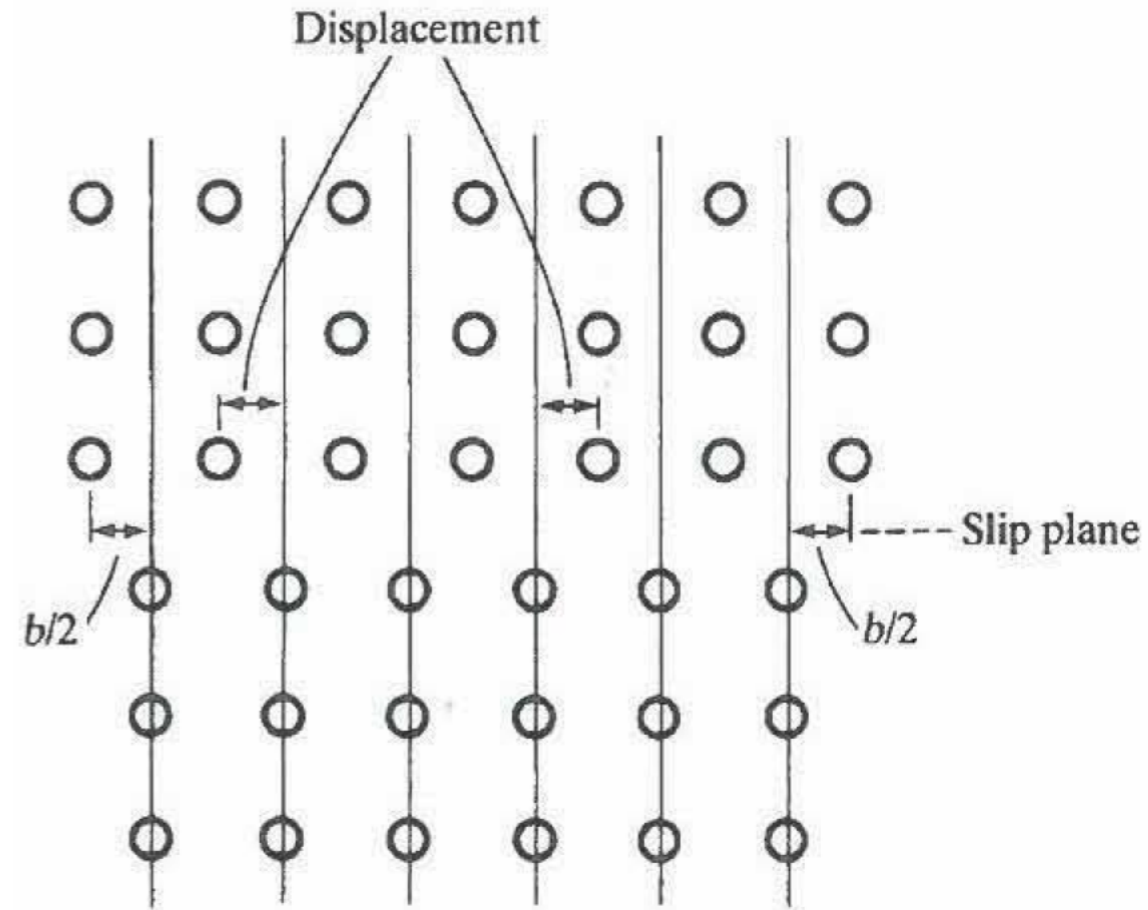
- Dislocation motion
- Peach-Koehler force
- Stress field of a dislocation
- Energy of a dislocation

Dislocation properties

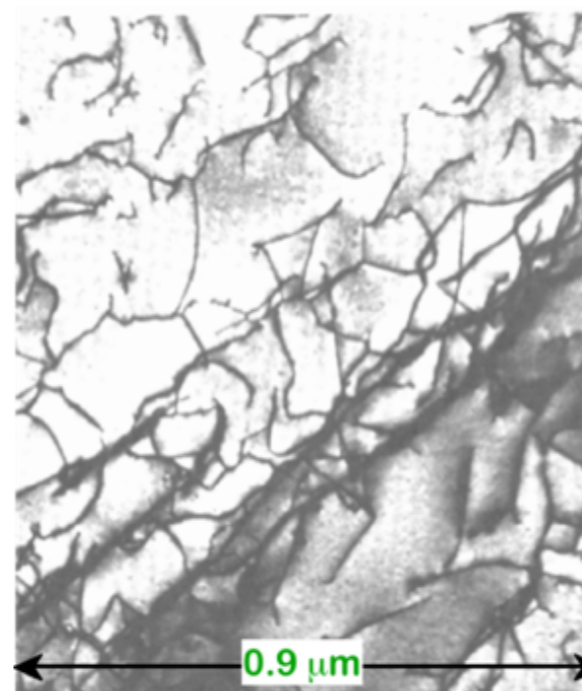
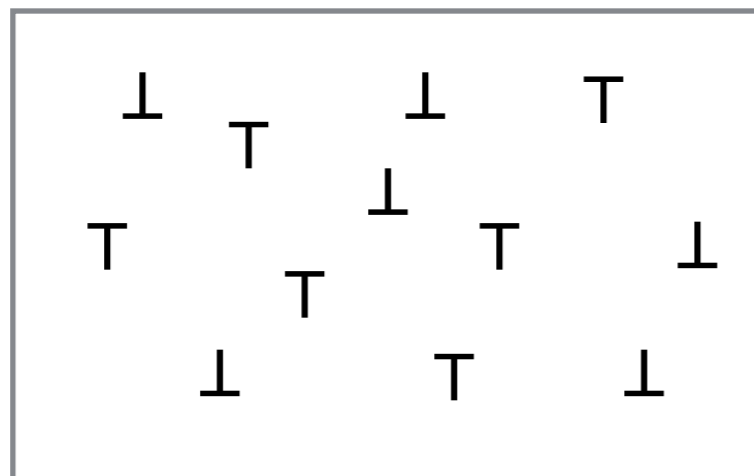
- Stress to move a dislocation: "lattice friction stress" or "Peierls stress"

$$\tau_f = G \exp \left[-\frac{2\pi w}{b} \right]$$

$w = b$	$\tau_f = 1.9 \times 10^{-3} G$
$w = 2b$	$\tau_f = 3.5 \times 10^{-6} G$
$w = 3b$	$\tau_f = 6.6 \times 10^{-9} G$

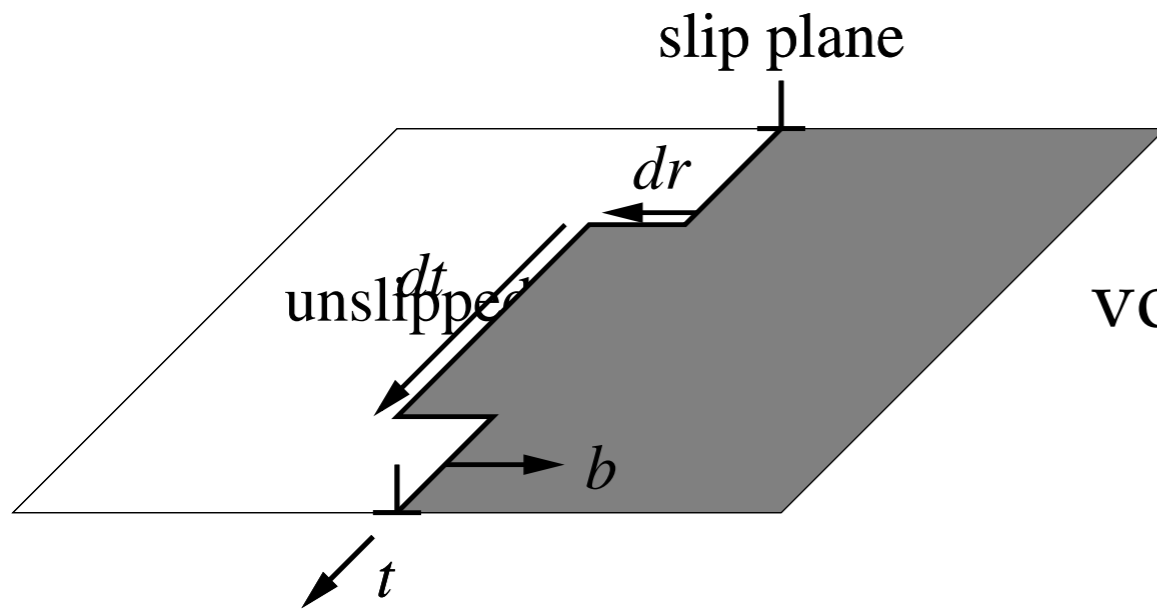


- Dislocation density:
 - # of dislocations per area
 - typically $\sim 10^{10} - 10^{14} \text{ m}^{-2}$
 - mean dislocation distance $\sim \rho^{-1/2}$



Quantifying dislocation motion

- Dislocation line: separates “slipped” from “unslipped” parts of crystal
 - Displacement of top and bottom half; **slip plane** divides top and bottom
 - Slip: bottom displaced by **b** relative to top
 - Both line direction **t** and Burgers vector **b** in slip plane



area swept: $d\mathbf{a} = d\mathbf{r} \times d\mathbf{t}$

volume change:
$$\begin{aligned}
 -\mathbf{b} \cdot d\mathbf{a} &= \mathbf{b} \cdot (d\mathbf{r} \times d\mathbf{t}) \\
 &= -(d\mathbf{r} \times d\mathbf{t}) \cdot \mathbf{b} \\
 &= -(d\mathbf{t} \times \mathbf{b}) \cdot d\mathbf{r}
 \end{aligned}$$

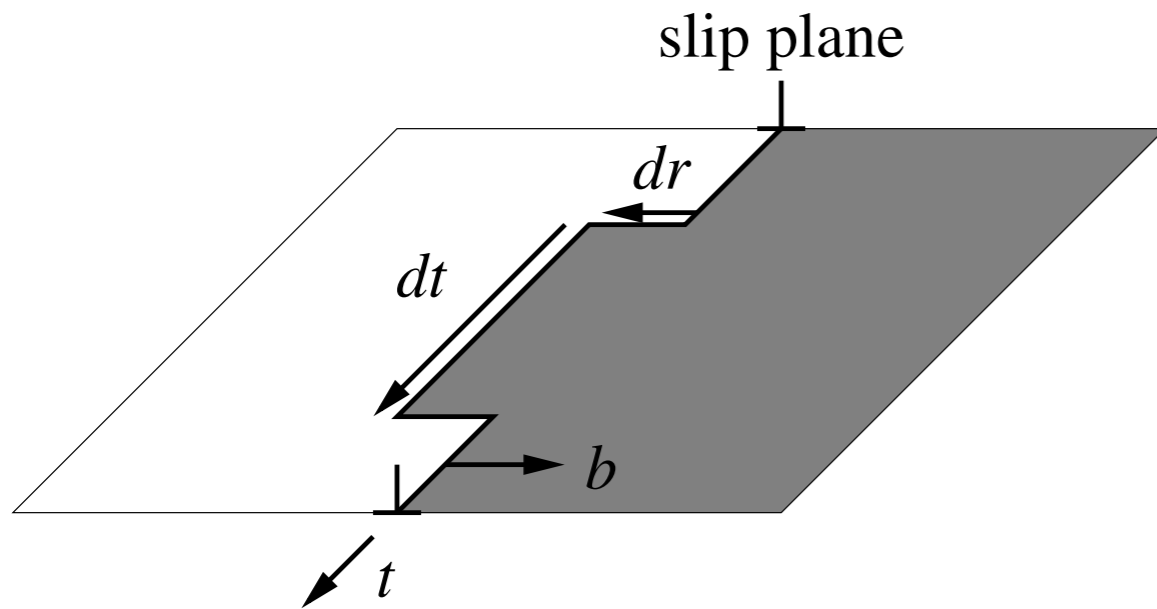
$dV = 0$ $d\mathbf{t} \times \mathbf{b} = 0$ or
 $d\mathbf{r} \cdot \mathbf{n} = 0$

glide

$dV \neq 0$ $-(d\mathbf{t} \times \mathbf{b}) \cdot d\mathbf{r} = -(\# \text{ vacancies}) \cdot (\text{volume per atom})$ **climb**

Dislocation motion under stress

- Dislocation line: separates “slipped” from “unslipped” parts of crystal
 - Sweeping out area displaces top part of crystal
 - Force on top area times displacement = –work done on dislocation



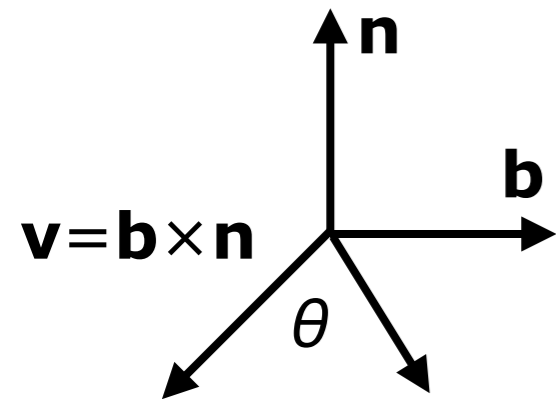
$$\mathbf{dF} = (\underline{\sigma} \cdot \mathbf{b}) \times \mathbf{dt}$$

Force/length on a dislocation

$$\begin{aligned} dW &= -(\text{force}) \cdot (\text{displacement}) \\ &= -(\text{stress} \cdot \text{area}) \cdot (\text{displacement}) \\ &= (\underline{\sigma} \cdot \mathbf{da}) \cdot \mathbf{b} = \mathbf{da} \cdot \underline{\sigma} \cdot \mathbf{b} \\ &= (\mathbf{dr} \times \mathbf{dt}) \cdot \underline{\sigma} \cdot \mathbf{b} \\ &= -(\mathbf{dt} \times \mathbf{dr}) \cdot (\underline{\sigma} \cdot \mathbf{b}) \\ &= -\left[(\underline{\sigma} \cdot \mathbf{b}) \times \mathbf{dt} \right] \cdot \mathbf{dr} \\ &= -\mathbf{dF} \cdot \mathbf{dr} \end{aligned}$$

Dislocation motion under stress

- Force per length (“Peach-Kohler force”)
 - Always perpendicular to dislocation line
 - Force **in slip plane**: *glide force*
 - Force **normal to slip plane**: *climb force* (edge) or *cross-slip* (screw)



$$\mathbf{t} = \mathbf{v} \cos \theta + \mathbf{b} \sin \theta$$

glide force

cross-slip force

climb force

$$d\mathbf{F} = (\underline{\sigma} \cdot \mathbf{b}) \times d\mathbf{t}$$

$$= \begin{pmatrix} \sigma_{vv} & \sigma_{vb} & \sigma_{vn} \\ \sigma_{vb} & \sigma_{bb} & \sigma_{bn} \\ \sigma_{vn} & \sigma_{bn} & \sigma_{nn} \end{pmatrix} \cdot \begin{pmatrix} 0 \\ b \\ 0 \end{pmatrix} \times \begin{pmatrix} \cos \theta \\ \sin \theta \\ 0 \end{pmatrix} dt$$

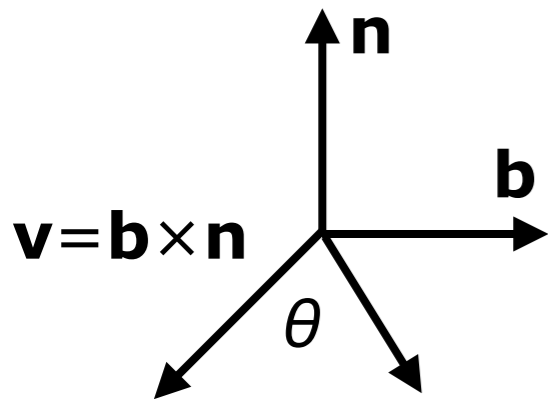
$$= \begin{pmatrix} \sigma_{bv}b \\ \sigma_{bb}b \\ \sigma_{bn}b \end{pmatrix} \times \begin{pmatrix} \cos \theta \\ \sin \theta \\ 0 \end{pmatrix} dt$$

$$= \begin{vmatrix} \mathbf{v} & \mathbf{b} & \mathbf{n} \\ \sigma_{bv}b & \sigma_{bb}b & \sigma_{bn}b \\ \cos \theta & \sin \theta & 0 \end{vmatrix} dt$$

$$= \sigma_{bn}b(-\mathbf{v} \sin \theta + \mathbf{b} \cos \theta) + \sigma_{bv}b \sin \theta \mathbf{n} - \sigma_{bb}b \cos \theta \mathbf{n}$$

Force on an edge and screw dislocation

- Force per length (“Peach-Kohler force”)
 - Always perpendicular to dislocation line
 - Force **in slip plane**: *glide force*
 - Force **normal to slip plane**: *climb force* (edge) or *cross-slip* (screw)



$$\mathbf{t} = \mathbf{v} \cos \theta + \mathbf{b} \sin \theta$$

$$\begin{aligned} d\mathbf{F} = & \sigma_{bn} b (-\mathbf{v} \sin \theta + \mathbf{b} \cos \theta) \\ & + \sigma_{bv} b \sin \theta \mathbf{n} - \sigma_{bb} b \cos \theta \mathbf{n} \end{aligned}$$

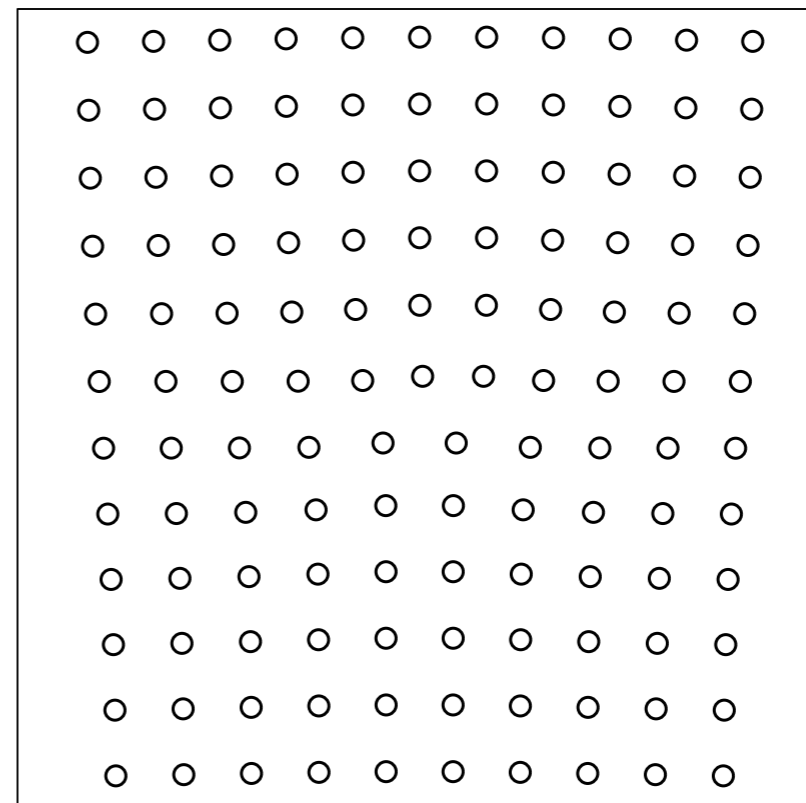
$$d\mathbf{F}_{\text{edge}} = \sigma_{bn} b \mathbf{b} - \sigma_{bb} b \mathbf{n}$$

$$d\mathbf{F}_{\text{screw}} = -\sigma_{bn} b \mathbf{v} + \sigma_{bv} b \mathbf{n}$$

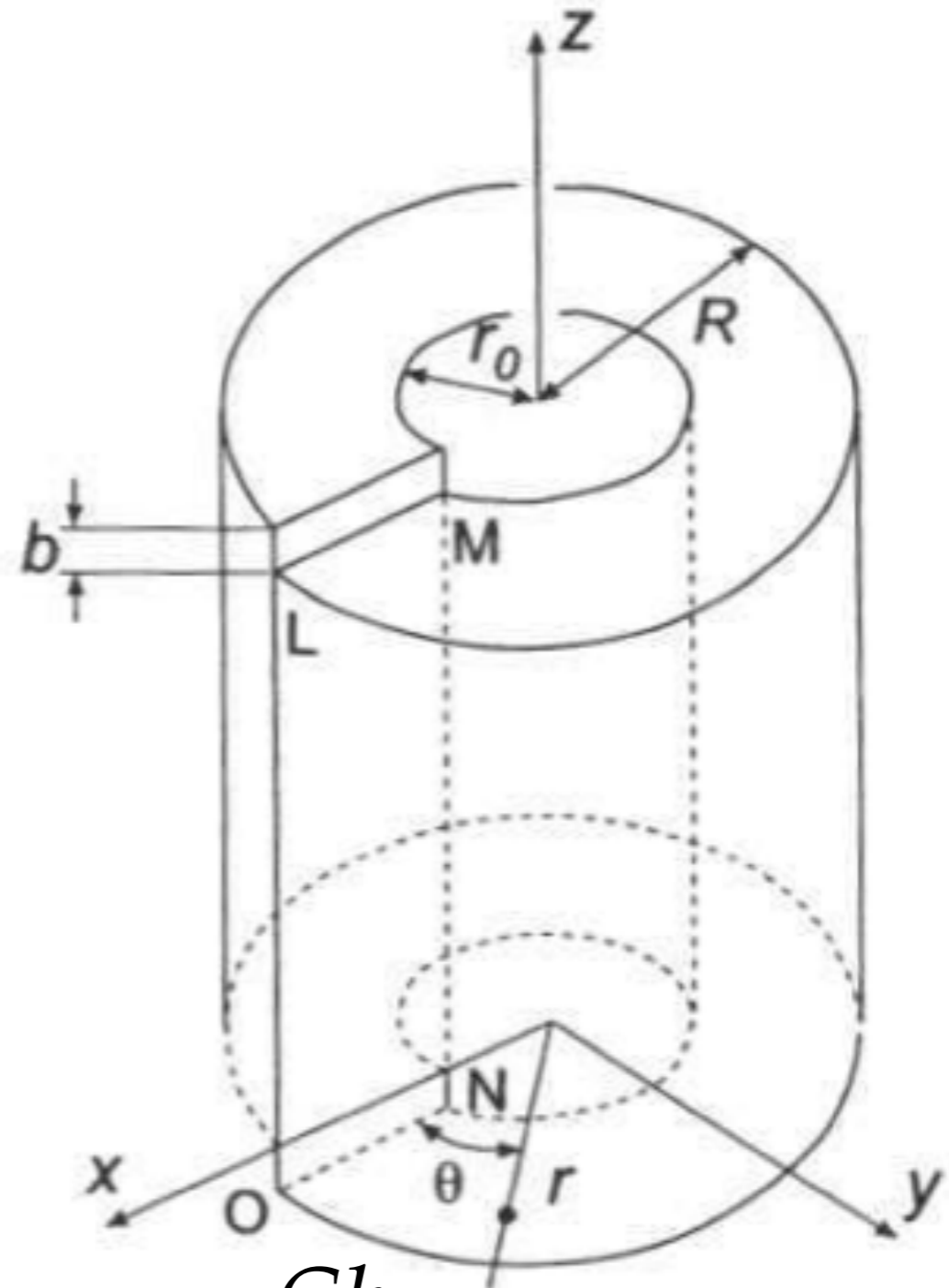
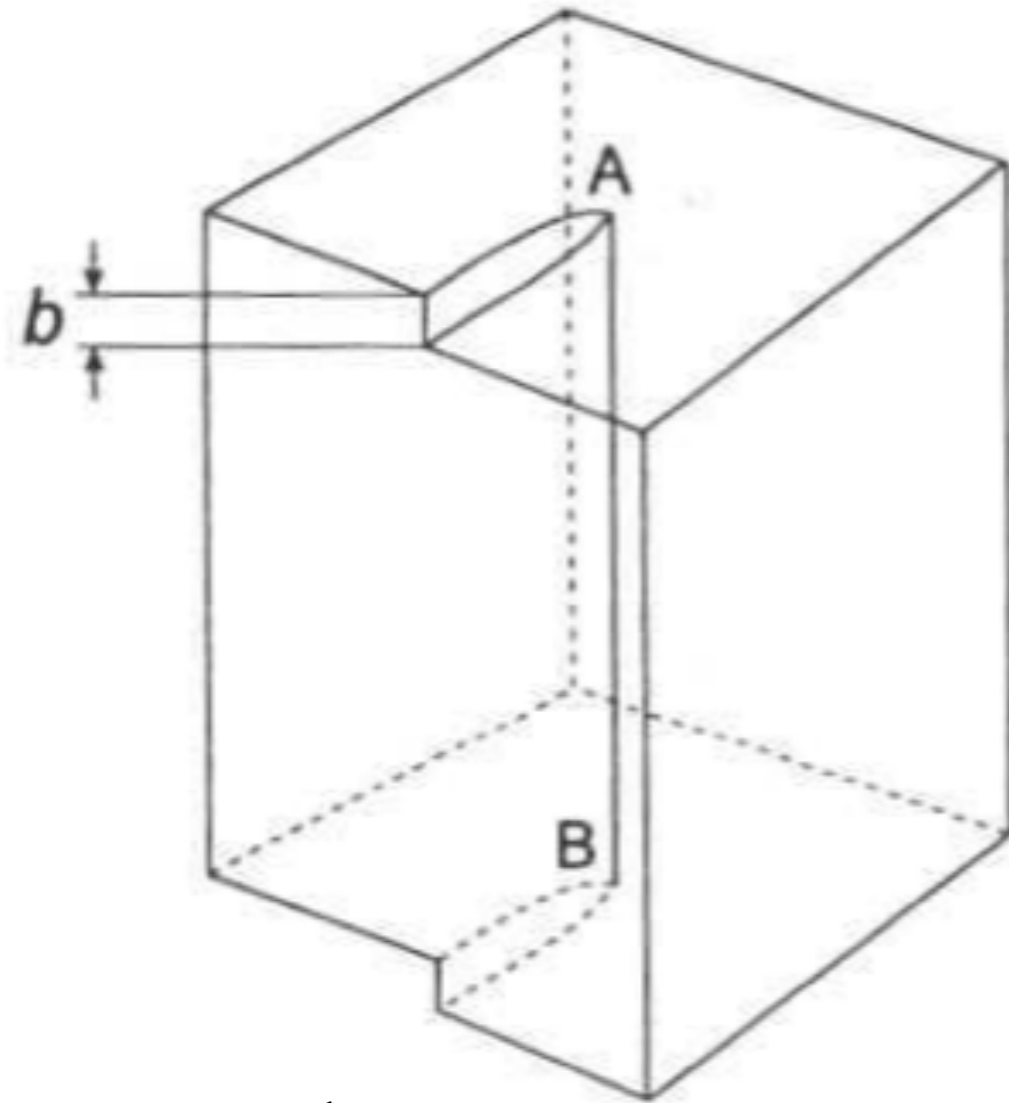
glide force

cross-slip force

climb force



Screw dislocation: stress field



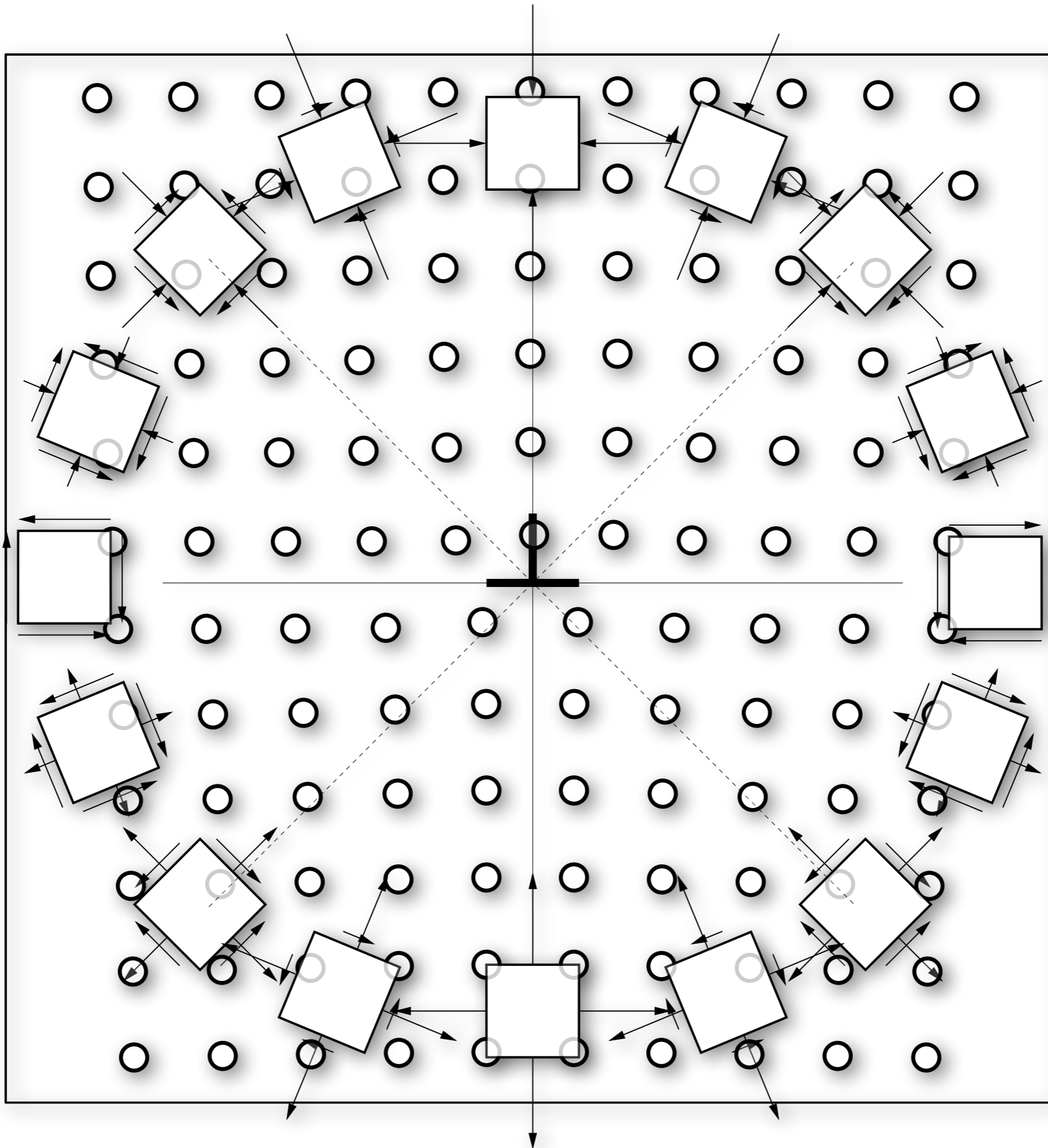
$$\gamma = \frac{b}{2\pi r}$$

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

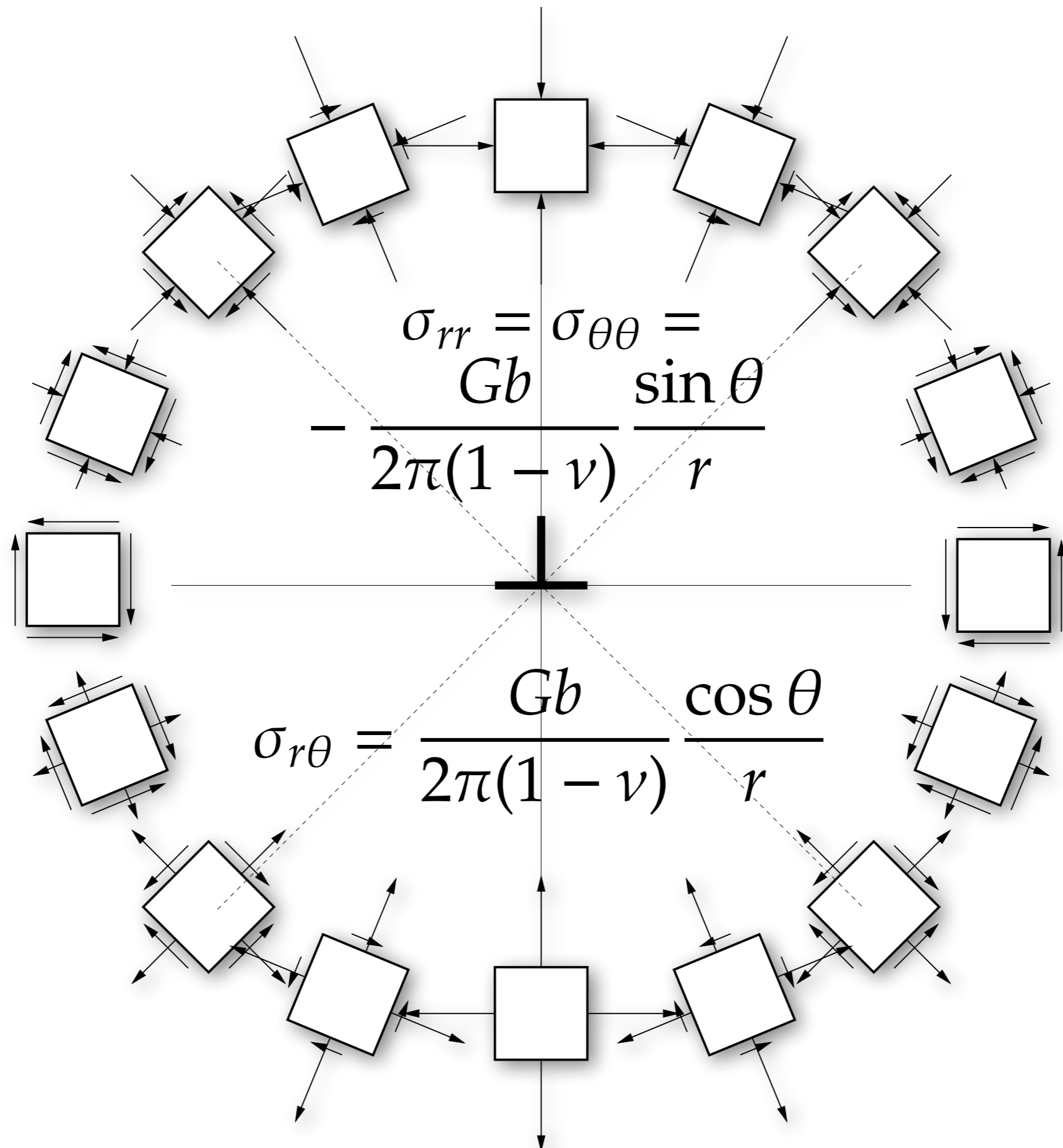
$$\sigma_{xz} = \sigma_{zx} = -\frac{Gb}{2\pi r} \sin \theta$$

$$\sigma_{yz} = \sigma_{zy} = \frac{Gb}{2\pi r} \cos \theta$$

Edge dislocation: stress field



Edge dislocation: stress field



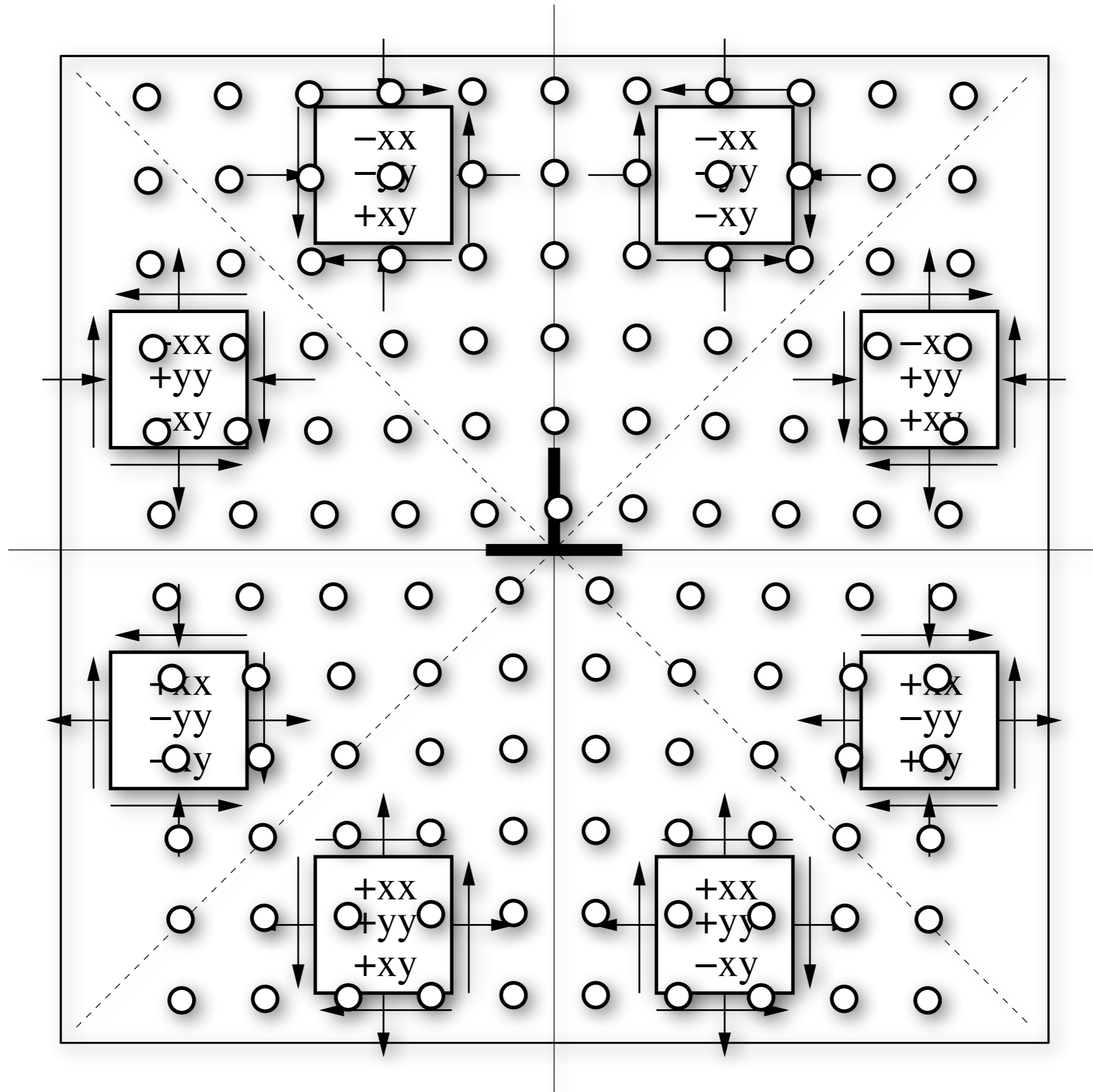
Edge dislocation: stress field

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

$$\theta_{\text{cart,polar}} = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$

$$\begin{aligned} \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{xy} & \sigma_{yy} \end{pmatrix} &= \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \sigma_{rr} & \sigma_{r\theta} \\ \sigma_{r\theta} & \sigma_{\theta\theta} \end{pmatrix} \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \\ &= \frac{Gb}{2\pi(1-\nu)r} \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} -\sin \theta & \cos \theta \\ \cos \theta & -\sin \theta \end{pmatrix} \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \\ &= \frac{Gb}{2\pi(1-\nu)r} \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} -2\sin \theta \cos \theta & -\sin^2 \theta + \cos^2 \theta \\ 1 & 0 \end{pmatrix} \\ &= \frac{Gb}{2\pi(1-\nu)r} \begin{pmatrix} -\sin \theta(1 + \cos^2 \theta) & \cos \theta \cos 2\theta \\ \cos \theta \cos 2\theta & -\sin \theta \cos 2\theta \end{pmatrix} \\ &= \frac{Gb}{2\pi(1-\nu)r} \begin{pmatrix} -\sin \theta(2 + \cos 2\theta) & \cos \theta \cos 2\theta \\ \cos \theta \cos 2\theta & -\sin \theta \cos 2\theta \end{pmatrix} \end{aligned}$$

Edge dislocation: stress field



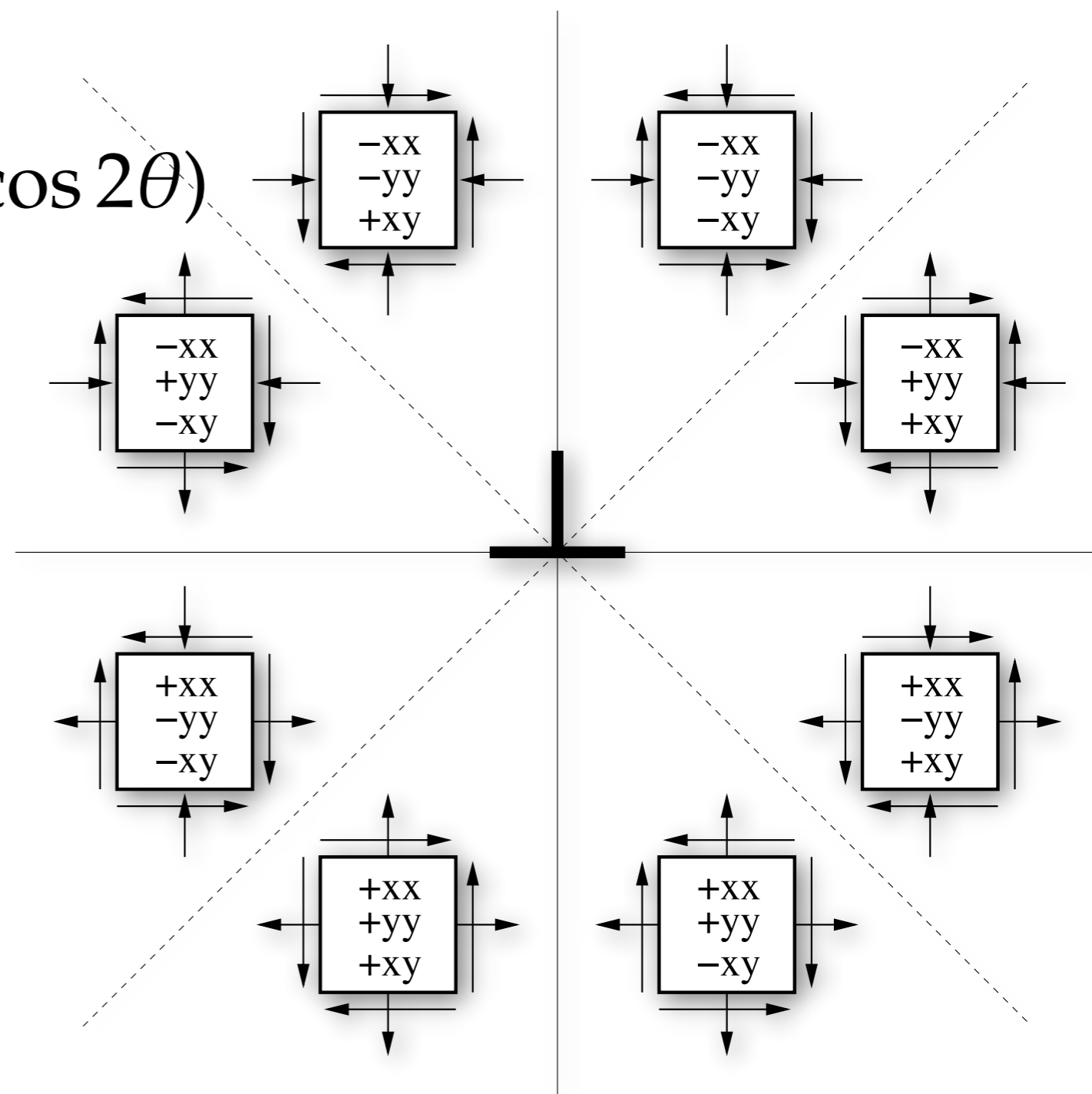
Edge dislocation: stress field

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

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

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

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

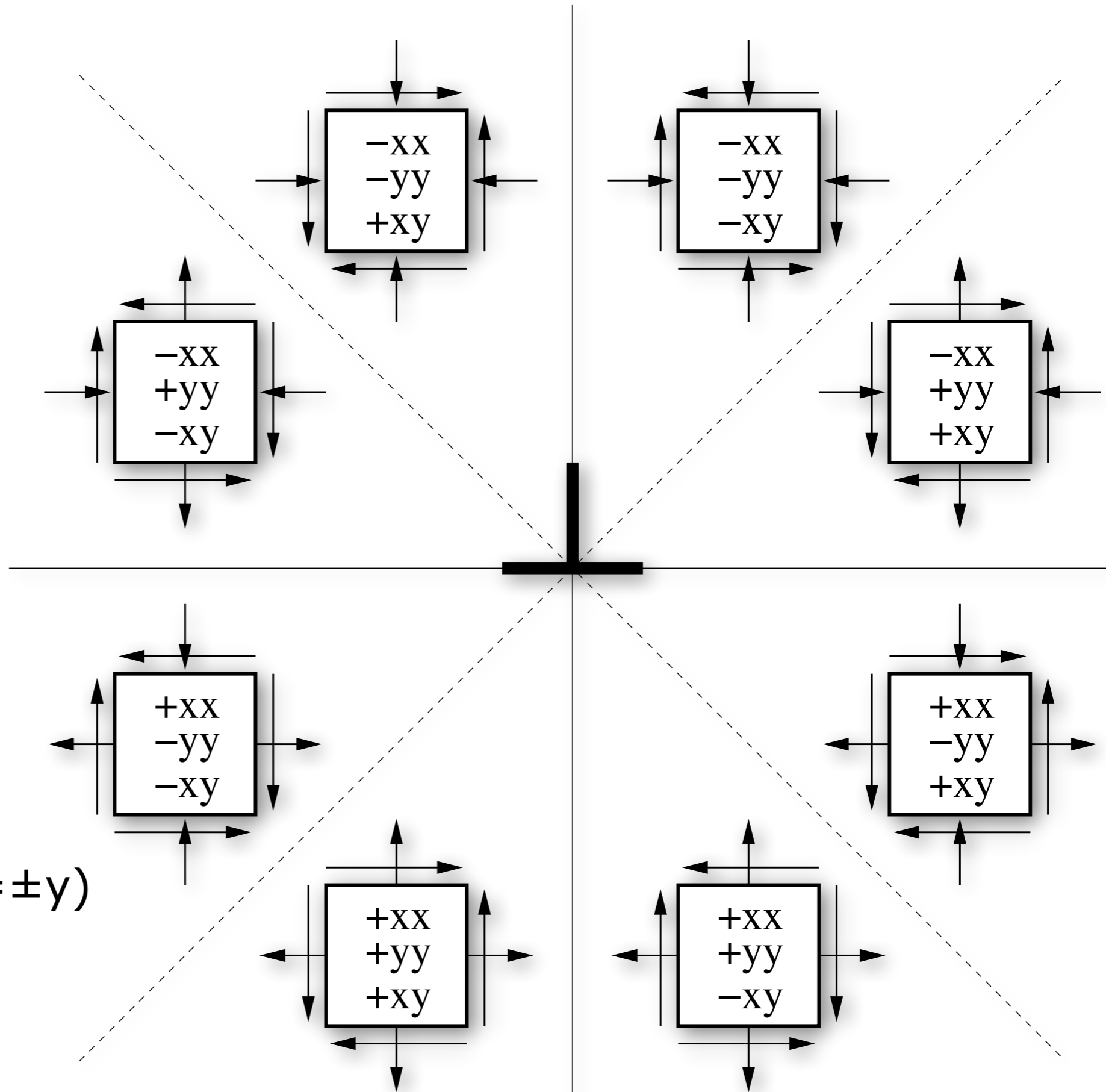


Edge dislocation: stress field

along **x axis** ($y=0$)
pure shear

along **y axis** ($x=0$)
pure compression
($y>0$)
pure tension
($y<0$)

along **diagonals** ($x=\pm y$)
only xx strain



Edge dislocation: stress field

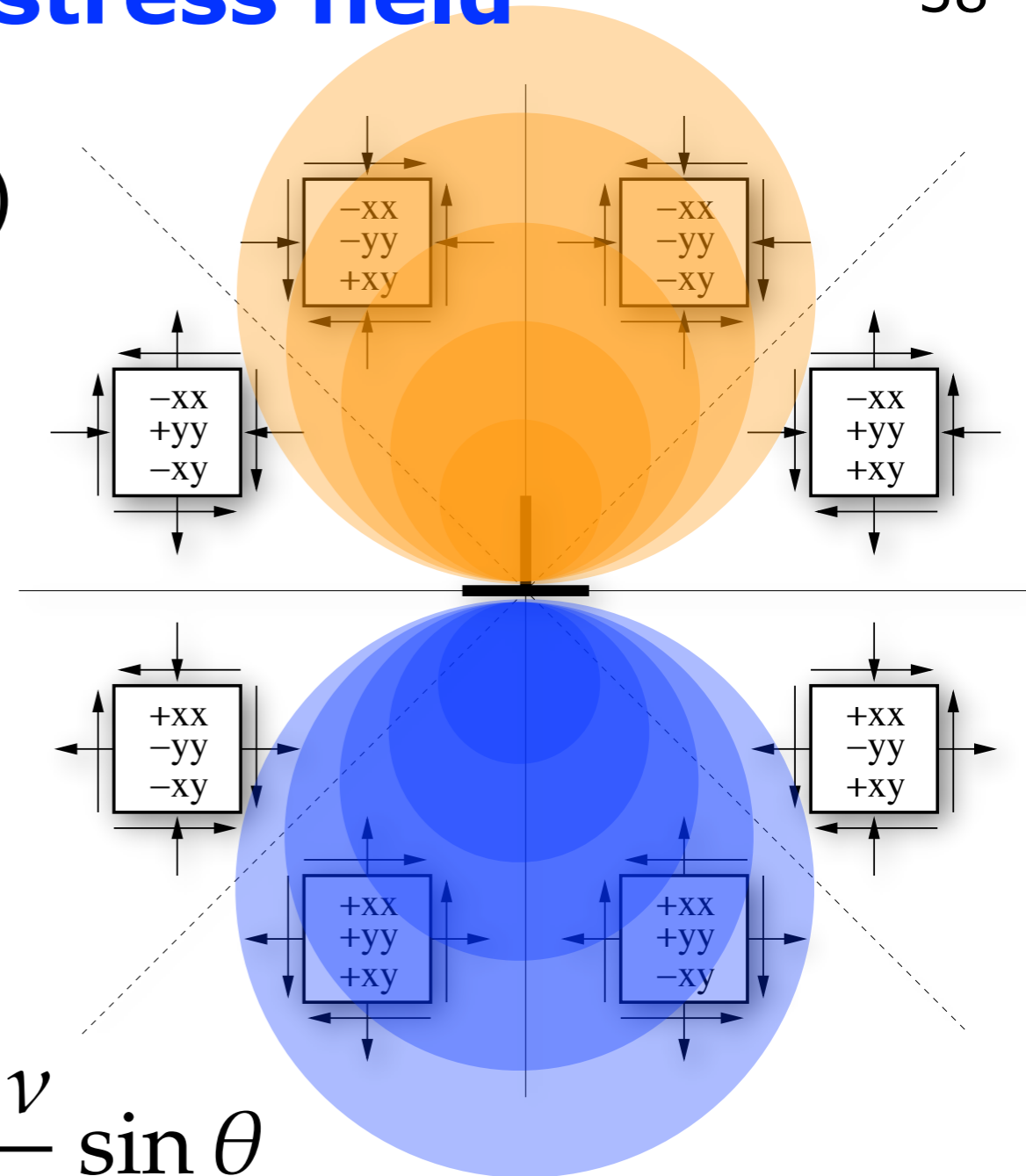
$$\sigma_{xx} = -\frac{Gb}{2\pi r(1-\nu)} \sin \theta (2 + \cos 2\theta)$$

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

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

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

$$\begin{aligned} p &= \frac{1}{3} (\sigma_{xx} + \sigma_{yy} + \sigma_{zz}) = -\frac{Gb}{3\pi r} \frac{1+\nu}{1-\nu} \sin \theta \\ &= -K \frac{b}{2\pi r} \frac{1-2\nu}{1-\nu} \sin \theta \\ &\approx -K \frac{b}{4\pi r} \sin \theta \end{aligned}$$



- Elastic energy per length: integrate elastic energy density

screw dislocation:

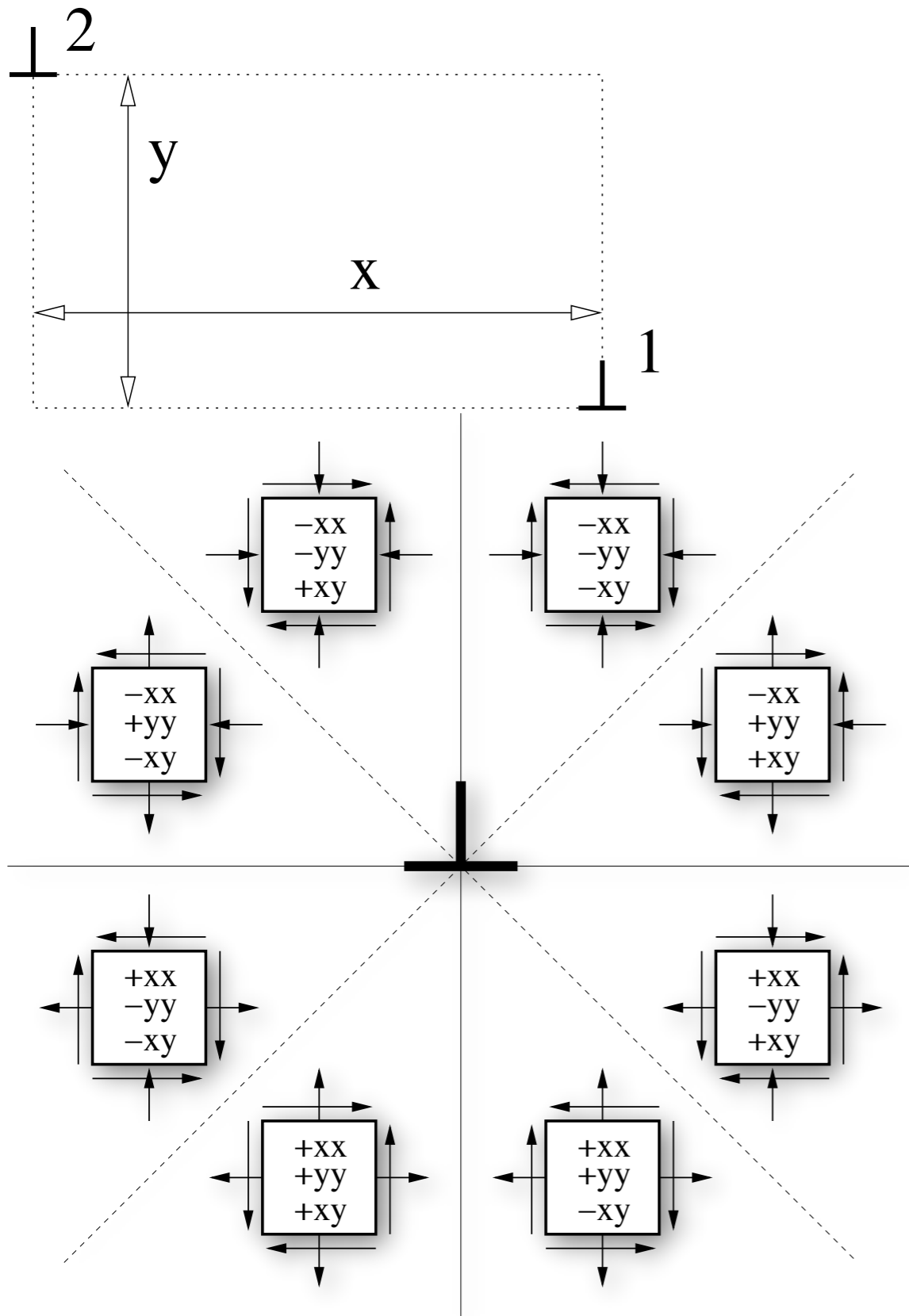
$$\begin{aligned}\frac{\text{energy}}{\text{length}} &= \int_{r_0}^{r_1} r \, dr \int_0^{2\pi} d\theta \frac{\tau^2}{2G} \\ &= \int_{r_0}^{r_1} r \, dr \frac{2\pi}{2G} \left(\frac{Gb}{2\pi r} \right)^2 \\ &= \frac{Gb^2}{4\pi} \int_{r_0}^{r_1} \frac{1}{r} \, dr \\ &= \frac{Gb^2}{4\pi} \ln \frac{r_1}{r_0} \approx \frac{1}{2} Gb^2\end{aligned}$$

edge dislocation:

$$\begin{aligned}\frac{\text{energy}}{\text{length}} &= \int_{r_0}^{r_1} r \, dr \int_0^{2\pi} d\theta \frac{1}{2} [\sigma_{rr}\epsilon_{rr} + \sigma_{\theta\theta}\epsilon_{\theta\theta} + \sigma_{r\theta}\epsilon_{r\theta}] \\ &= [\text{more integration...}] \\ &= \dots \\ &= \frac{Gb^2}{4\pi(1-\nu)} \ln \frac{r_1}{r_0} \approx \frac{1}{2(1-\nu)} Gb^2\end{aligned}$$

Dislocation/dislocation interaction

- Stress from edge dislocation 1 gives force on edge dislocation 2



$$\begin{aligned}
 \mathbf{F}_{21} &= \tau_{xy}^{(1)} b_2 \mathbf{i} - \sigma_{xx}^{(1)} b_2 \mathbf{j} \\
 &= \frac{Gb_1 b_2}{2\pi(1-\nu)r} \cos \theta \cos 2\theta \mathbf{i} \\
 &\quad + \frac{Gb_1 b_2}{2\pi(1-\nu)r} \sin \theta (2 + \cos 2\theta) \mathbf{j}
 \end{aligned}$$

- Dislocation motion
- Peach-Koehler force
- Stress field of a dislocation
- Energy of a dislocation

- Dislocations in particular crystal structures: FCC, BCC, HCP, intermetallics
- Kinks and dislocation mobility
- Dislocation intersections and jogs

Slip systems: FCC, BCC, and HCP

Crystal structure	Slip planes	Slip directions	Number of slip systems
Face-centered cubic	$\{111\} \times 4$	$\langle 1\bar{1}0 \rangle \times 3$	$4 \times 3 = 12$
Body-centered cubic	$\{110\} \times 6$	$\langle \bar{1}11 \rangle \times 2$	$6 \times 2 = 12$
	$\{211\} \times 12$	$\langle \bar{1}11 \rangle \times 1^*$	$12 \times 1 = 12$
	$\{321\} \times 24$	$\langle \bar{1}11 \rangle \times 1^*$	$24 \times 1 = 24$
Hexagonal-closed packed	$\{0001\} \times 1$	$\langle 11\bar{2}0 \rangle \times 3$	$1 \times 3 = 3$
	$\{10\bar{1}0\} \times 3$	$\langle 11\bar{2}0 \rangle \times 1$	$3 \times 1 = 3$
	$\{10\bar{1}1\} \times 6$	$\langle 11\bar{2}0 \rangle \times 1$	$6 \times 1 = 6$

*sign of slip direction important

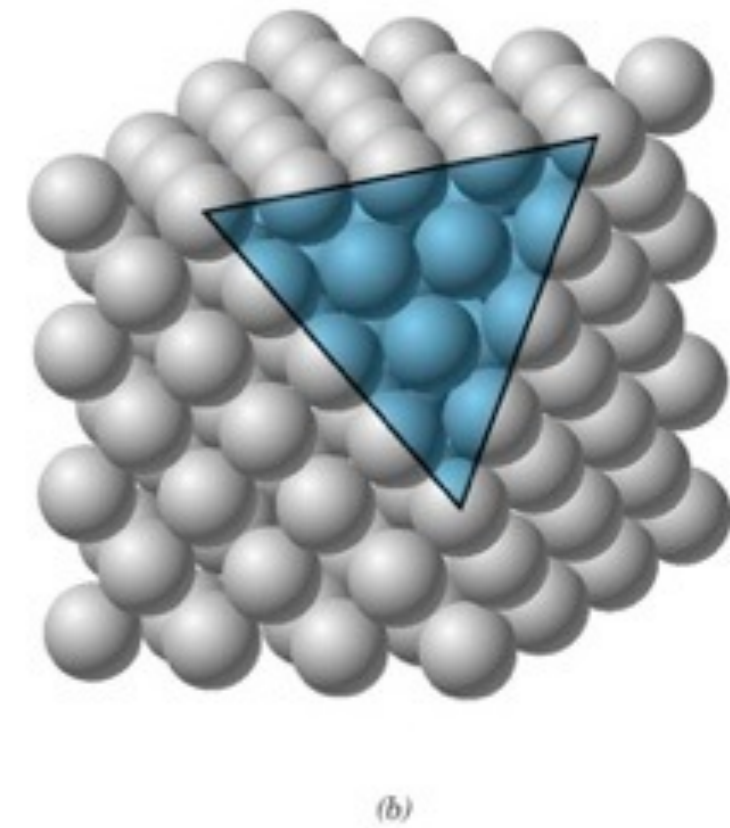
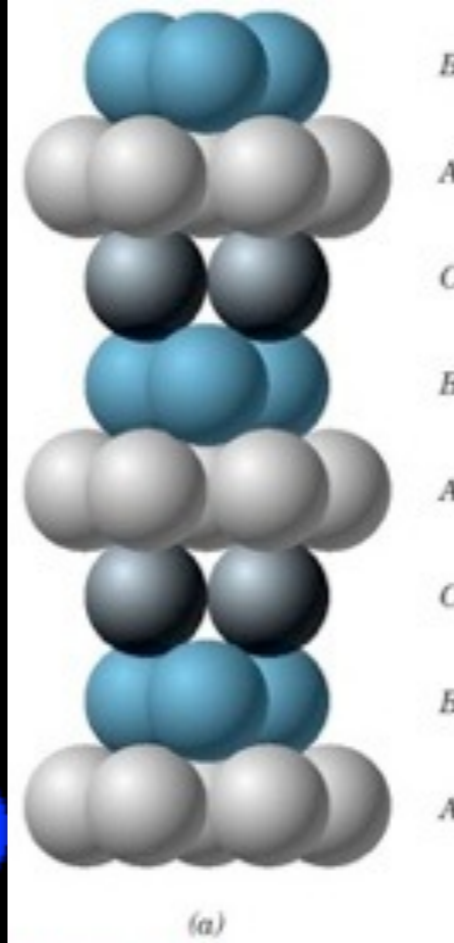
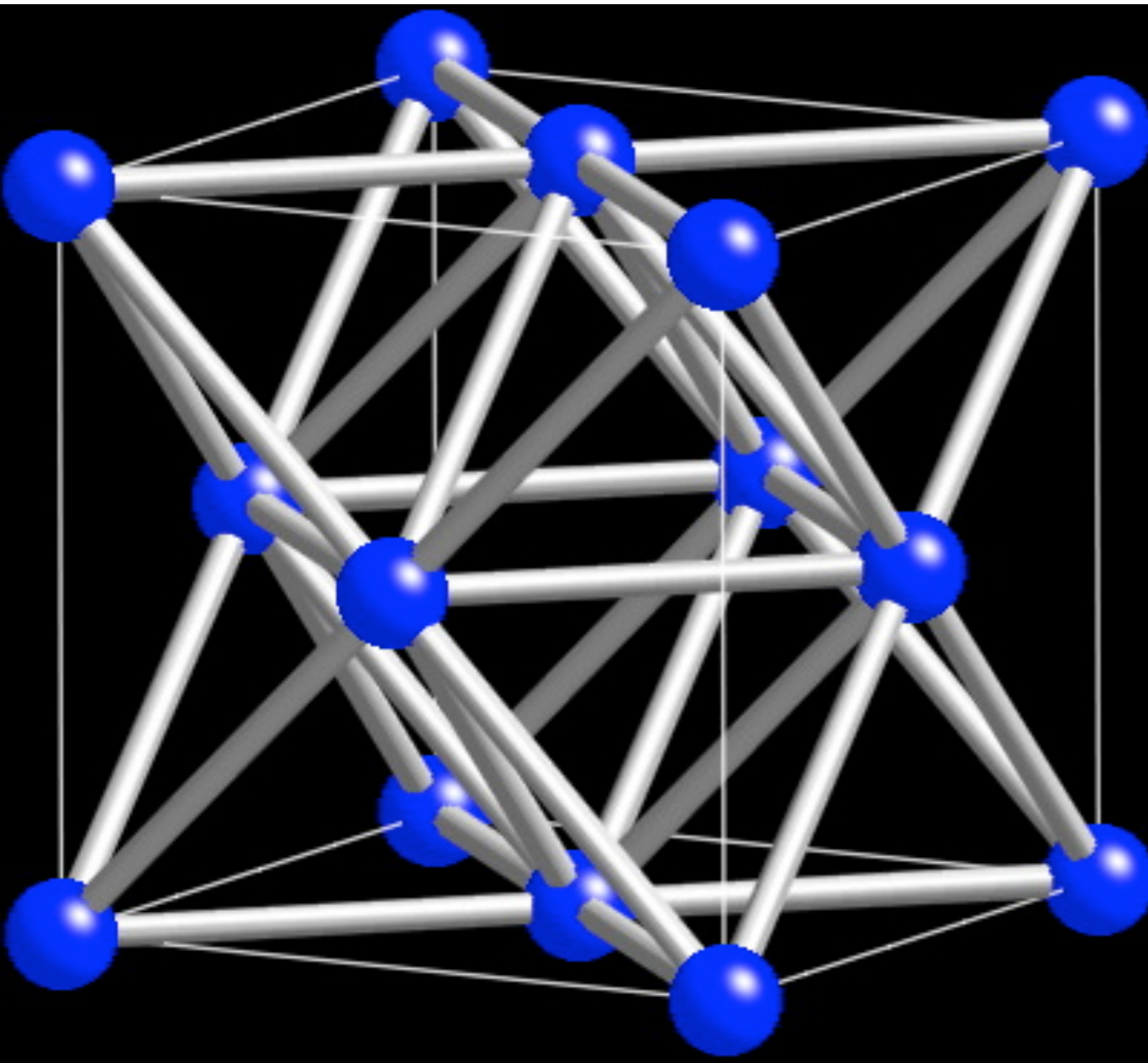
$$\underline{\varepsilon} = \gamma \begin{pmatrix} b_x n_x & \frac{1}{2}(b_x n_y + b_y n_x) & \frac{1}{2}(b_x n_z + b_z n_x) \\ \frac{1}{2}(b_y n_x + b_x n_y) & b_y n_y & \frac{1}{2}(b_y n_z + b_z n_y) \\ \frac{1}{2}(b_z n_x + b_x n_z) & \frac{1}{2}(b_z n_y + b_y n_z) & b_z n_z \end{pmatrix}$$

FCC: Al, Cu, Ni, Ag, Au ...

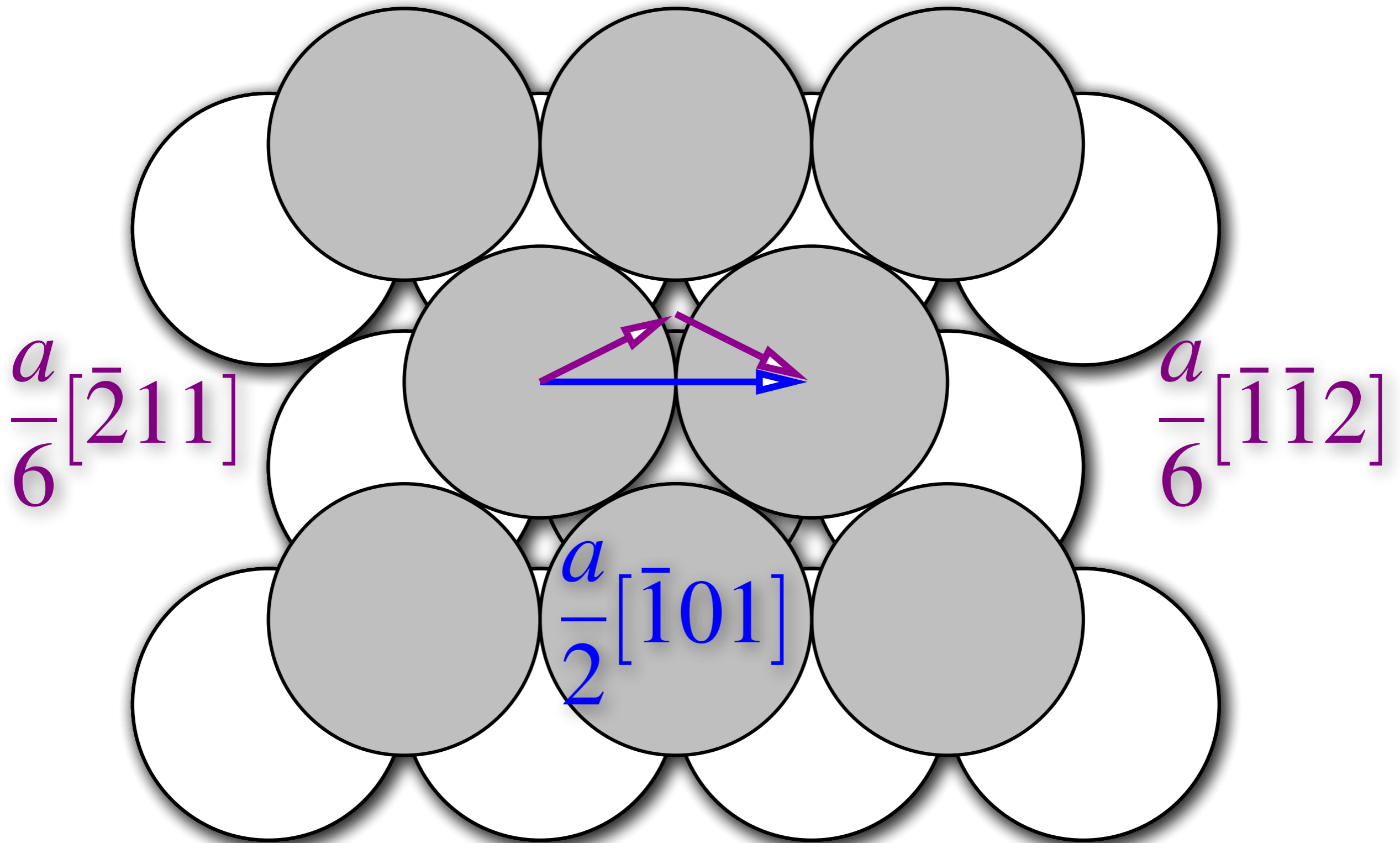
BCC: Fe, Nb, Mo, Ta, W ...

HCP: Zn, Cd, Mg, Ti, Zr ...

FCC crystal structure

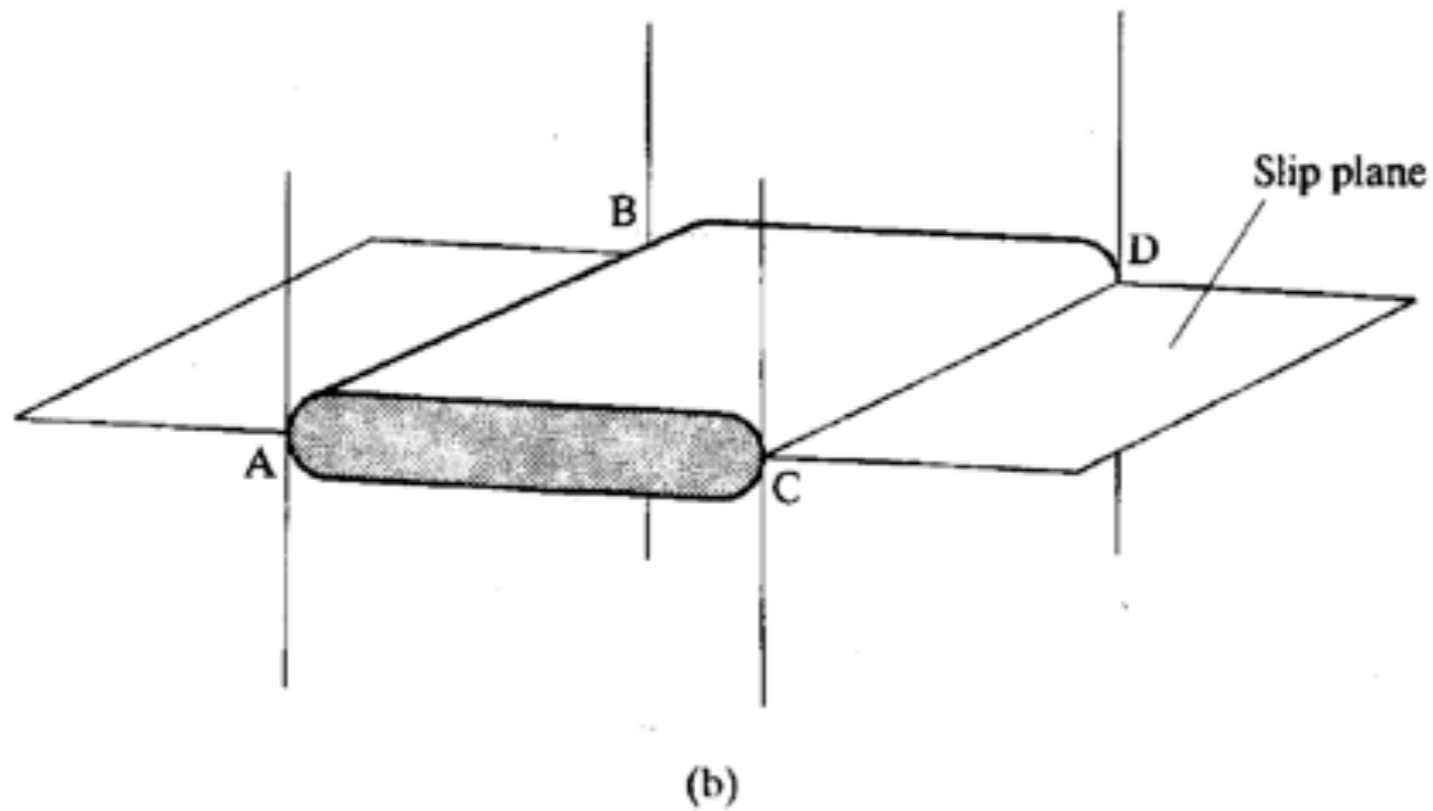
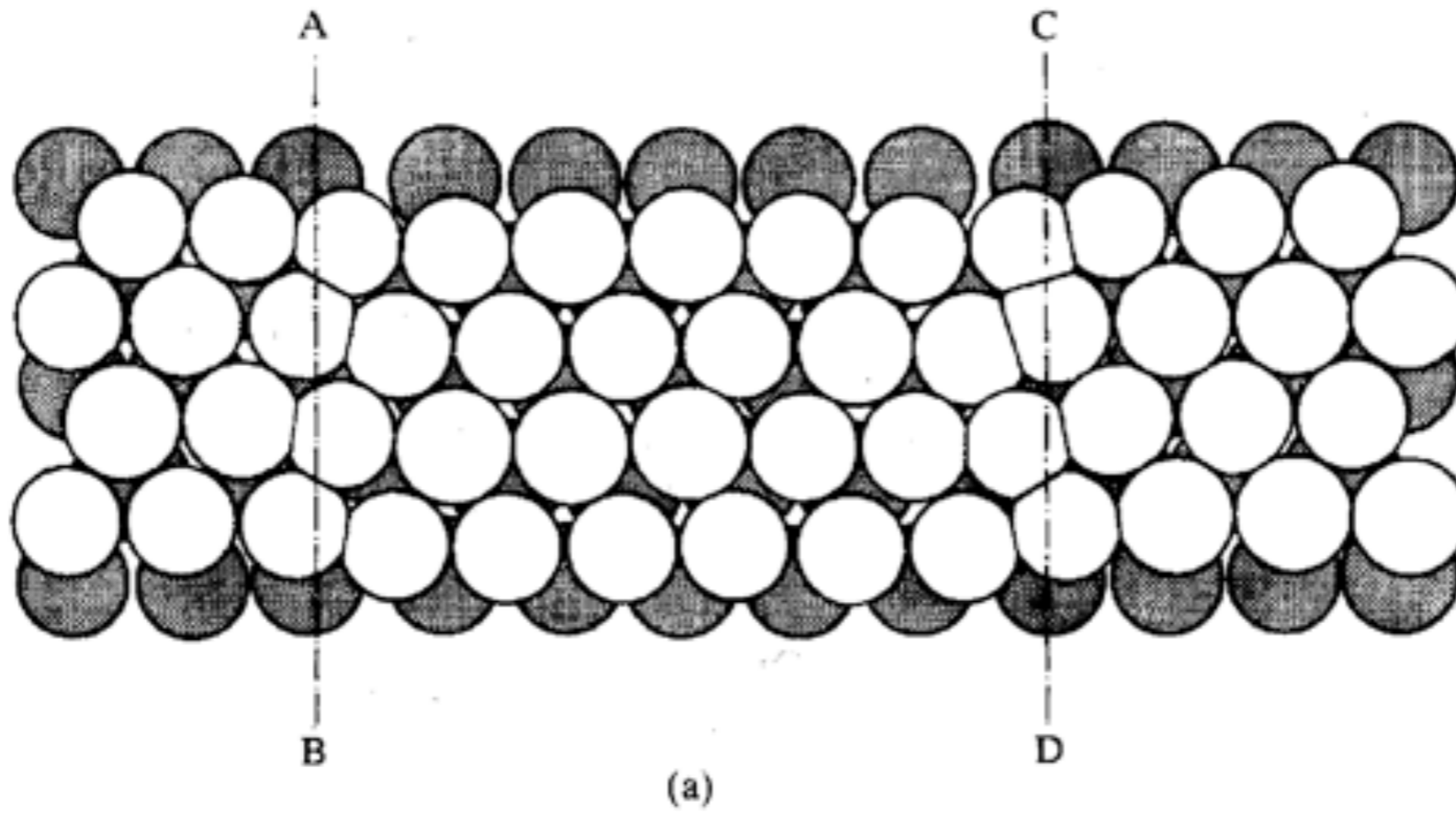


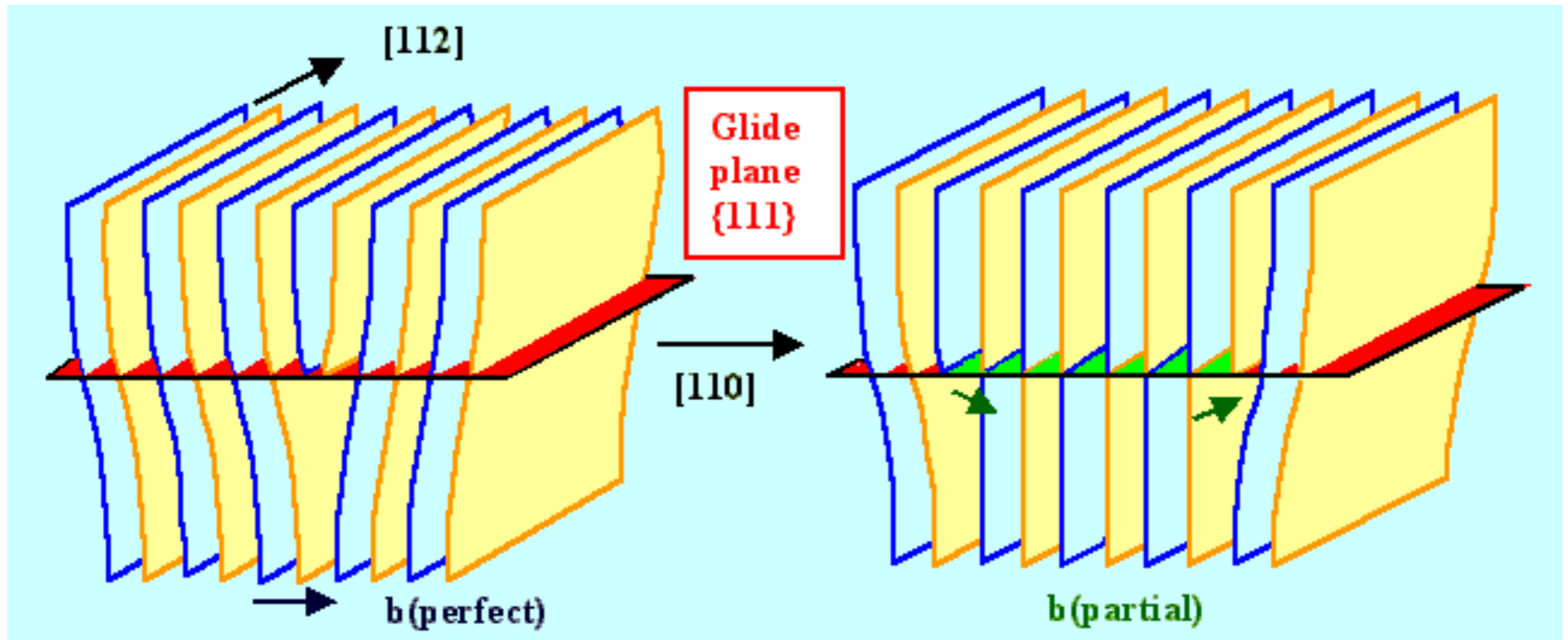
FCC stacking fault



(111) slip plane

FCC partial dislocations and stacking fault





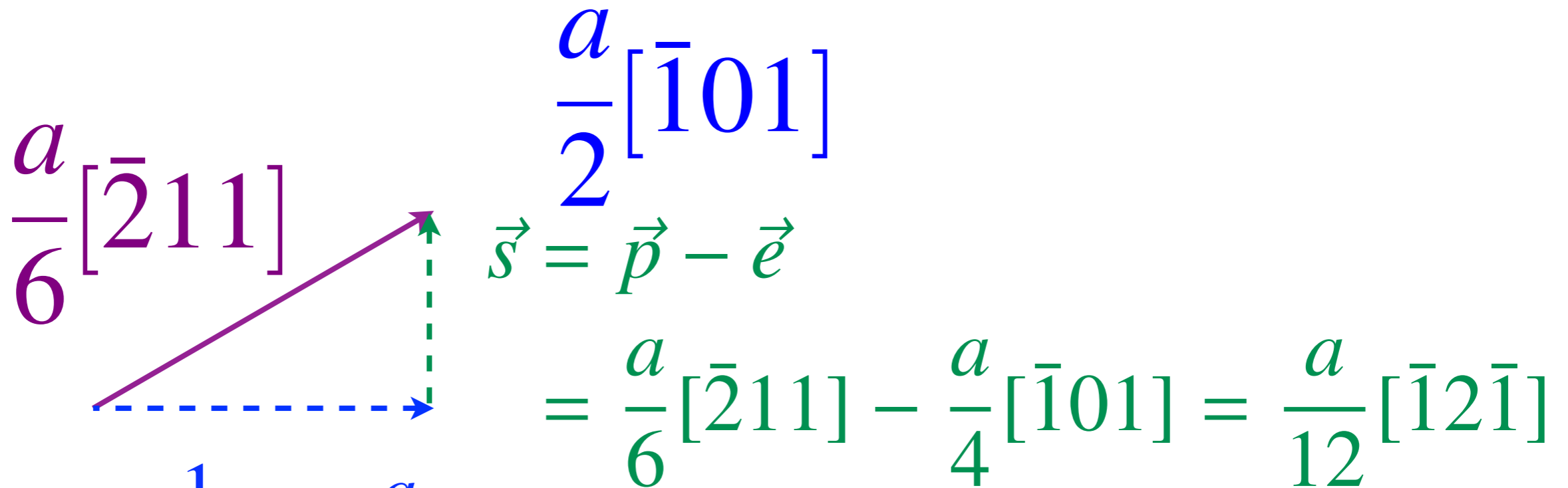
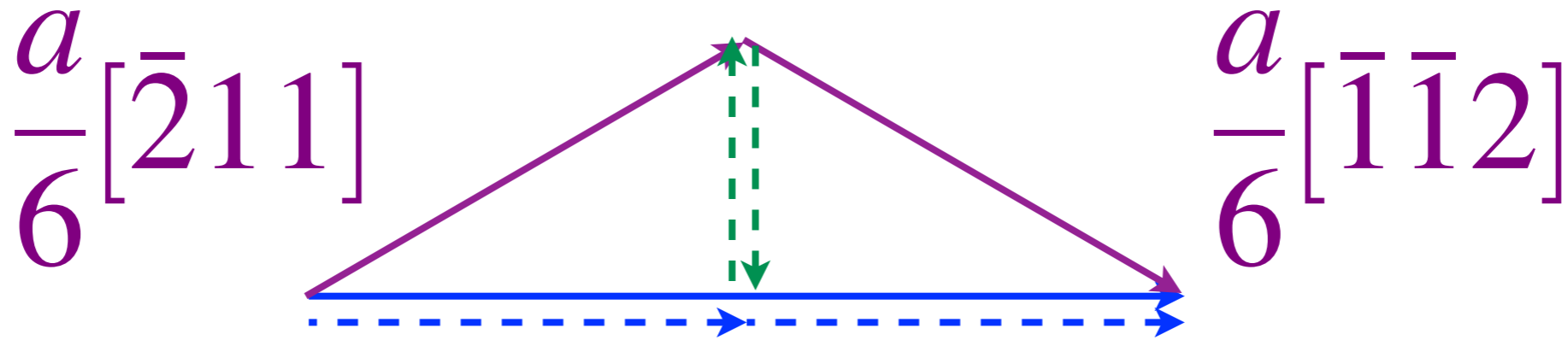
(110) planes “alternate” with an “1-2” stacking (blue=1, yellow=2).

perfect dislocation = new 1 and 2 planes;

each partial puts in a 1 (first partial) or 2 (second partial) plane.

N.B.: the ABC stacking is in each (110) plane—so every “1” plane has A, B, and C atoms, as does every “2” plane.

FCC partial splitting: geometry



$$\vec{e} = \frac{1}{2}\vec{b} = \frac{a}{4}[\bar{1}01]$$

$$e^2 = \frac{a^2}{16}(1 + 1 + 0) = \frac{a^2}{8}$$

$$s^2 = \frac{a^2}{144}(1 + 4 + 1) = \frac{a^2}{24}$$

threading direction

FCC partial splitting: geometry

$$0 = \mathbf{F}_{\text{int}} = \mathbf{F}_{\text{edge}} + \mathbf{F}_{\text{screw}} + \mathbf{F}_{\text{stacking fault}}$$
$$= \frac{Ge^2}{2\pi(1-\nu)d} - \frac{Gs^2}{2\pi d} - (\text{SFE})$$

$$e^2 = \frac{a^2}{16}(1 + 1 + 0) = \frac{a^2}{8}$$

$$s^2 = \frac{a^2}{144}(1 + 4 + 1) = \frac{a^2}{24}$$

$$(\text{SFE}) = \frac{Ga^2}{\pi d} \left[\frac{1}{16(1-\nu)} - \frac{1}{48} \right]$$

$$= \frac{Ga^2}{16\pi d} \left[\frac{2+\nu}{3(1-\nu)} \right]$$

$$\frac{2 + \frac{1}{3}}{3(1 - \frac{1}{3})} = \frac{7}{6} \approx 1$$

$$d_{\text{edge}} \approx \frac{Ga^2}{16\pi(\text{SFE})}$$

$$d_{\text{screw}} \approx \frac{Ga^2}{32\pi(\text{SFE})}$$

threading
direction

Partial splitting: material dependence

$$d_{\text{edge}} \approx \frac{Ga^2}{16\pi(\text{SFE})}$$

$$d_{\text{screw}} \approx \frac{Ga^2}{32\pi(\text{SFE})}$$

	SFE [mJ/m ²]	G [GPa]	a [nm]	d_{edge} [nm]
Al	200	27	0.405	0.441
Cu	40	48	0.362	3.13
Cu-7%Al	4	48	0.38	34.5

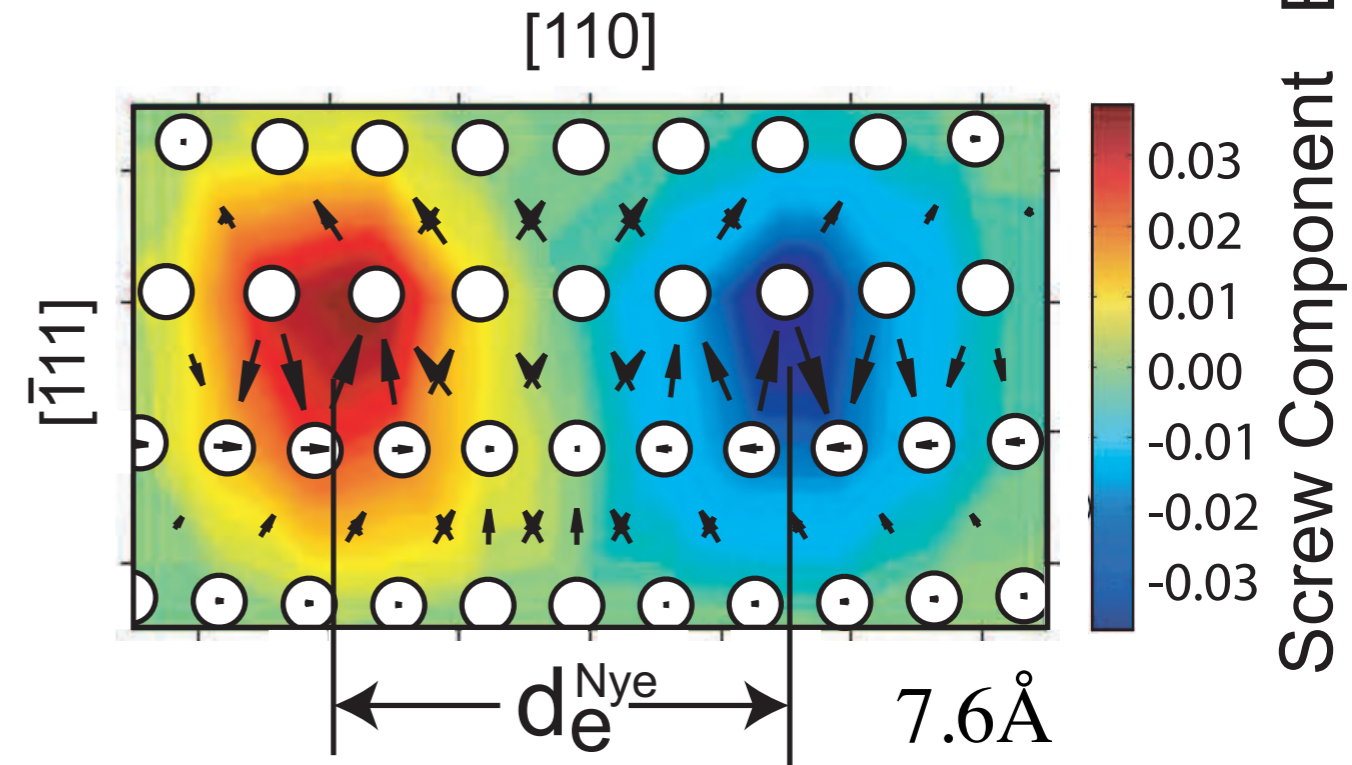
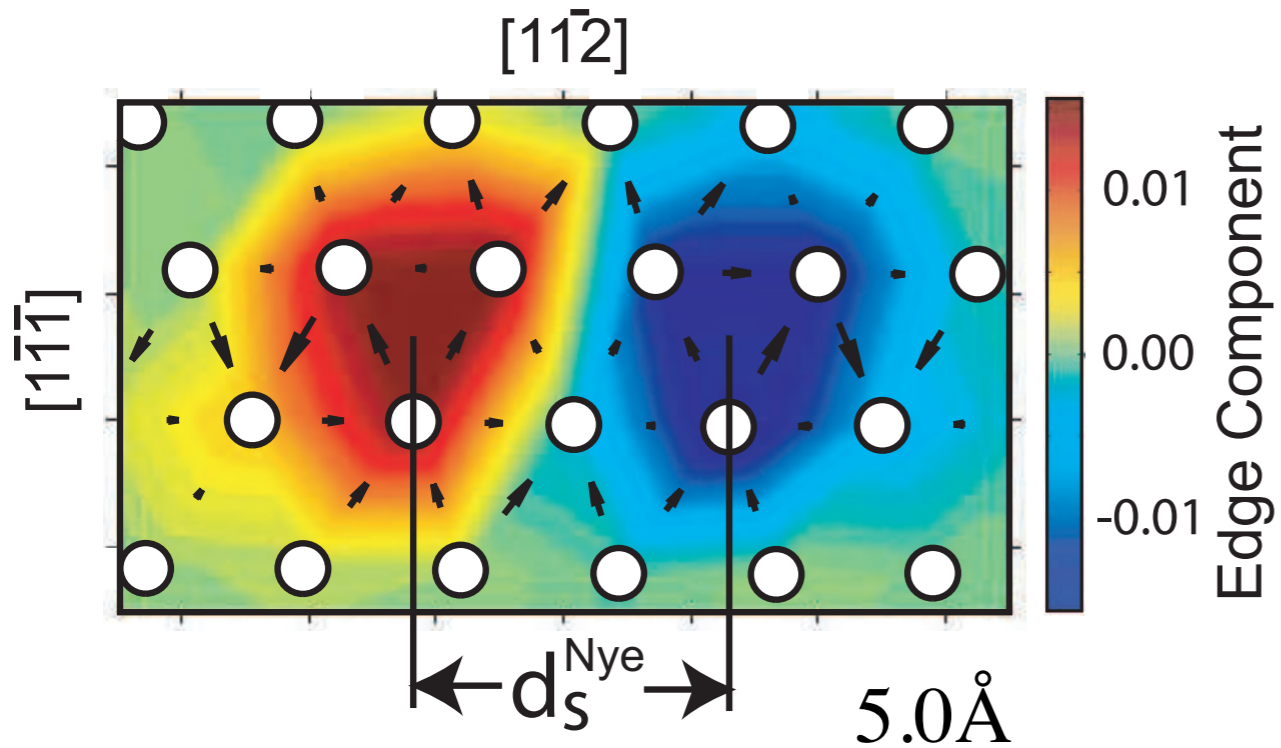
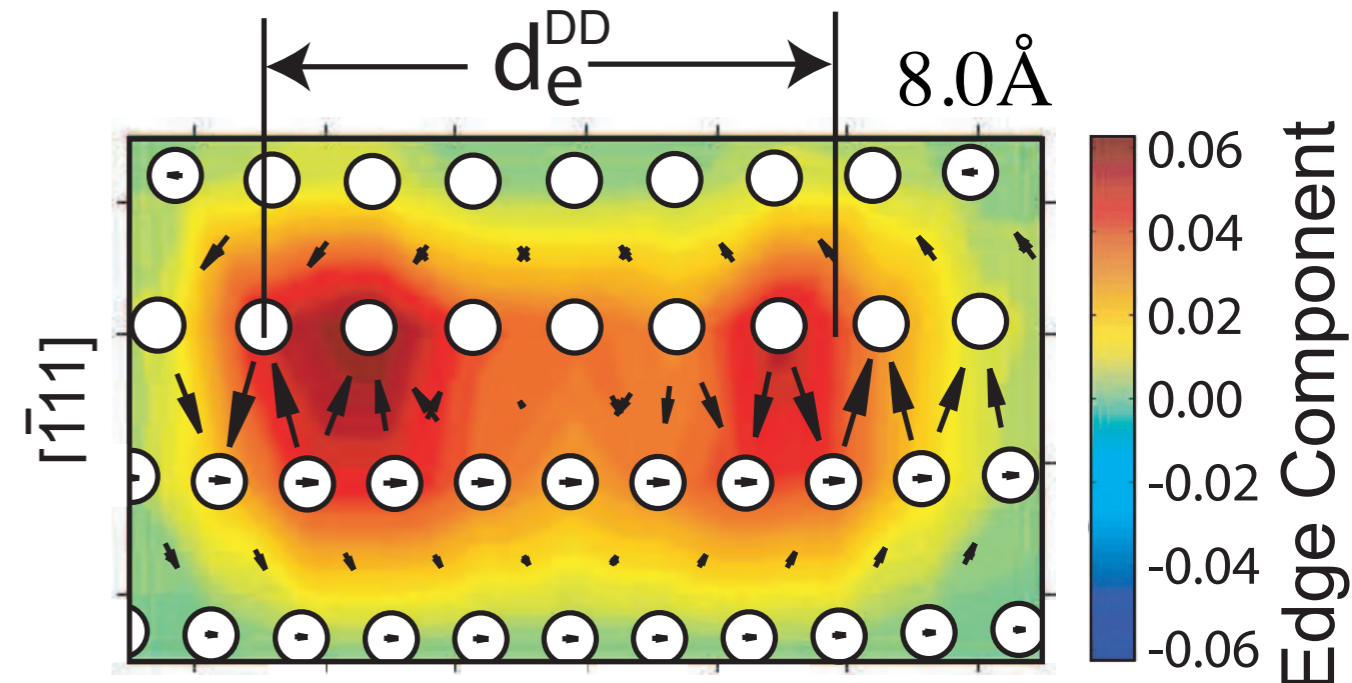
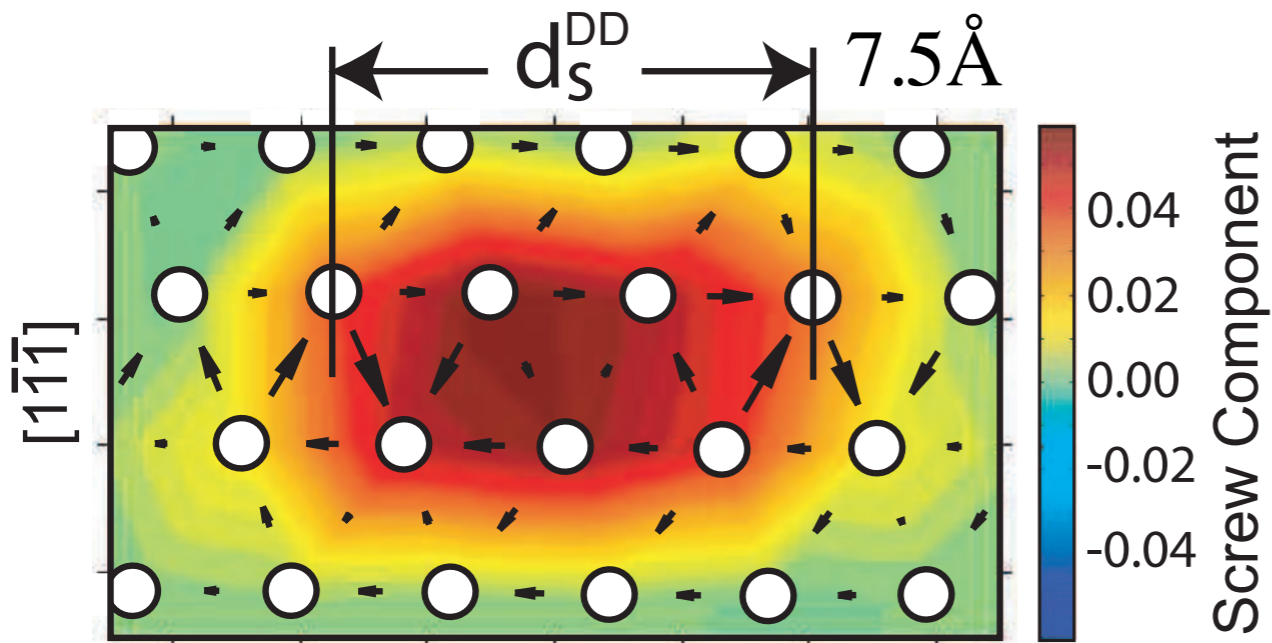
“low” v. “high” stacking fault energy =
large v. small splitting (relative to Burgers vector)
small splitting = easier cross-slip for screw dislocation

Aluminum dislocation cores: screw and edge 50

Differential displacement (arrows) and Nye tensor density (colors)

$a/2\langle 110 \rangle$ Edge Dislocation

$a/2\langle 110 \rangle$ Screw Dislocation



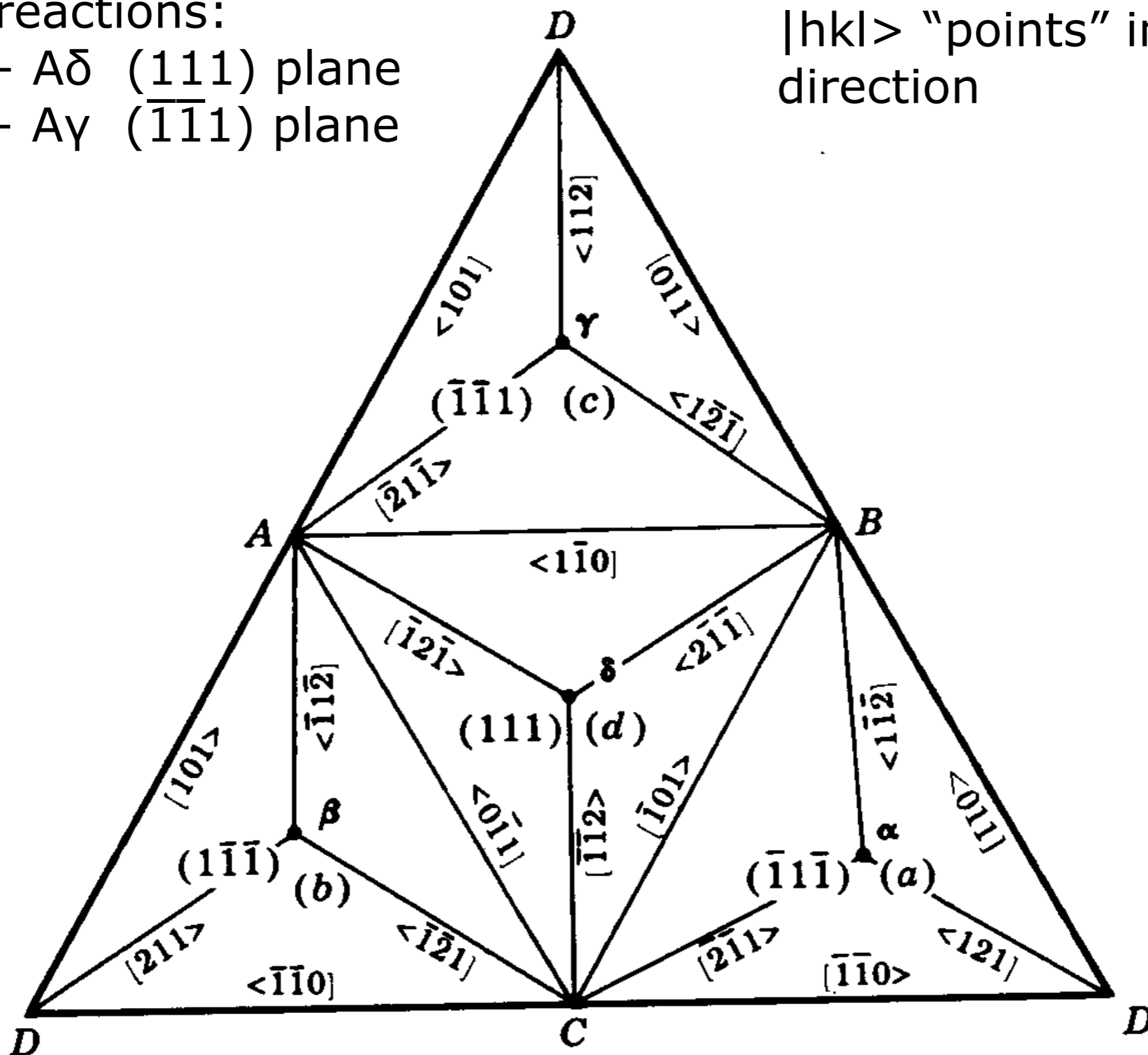
Thompson tetrahedron and partials

Example reactions:

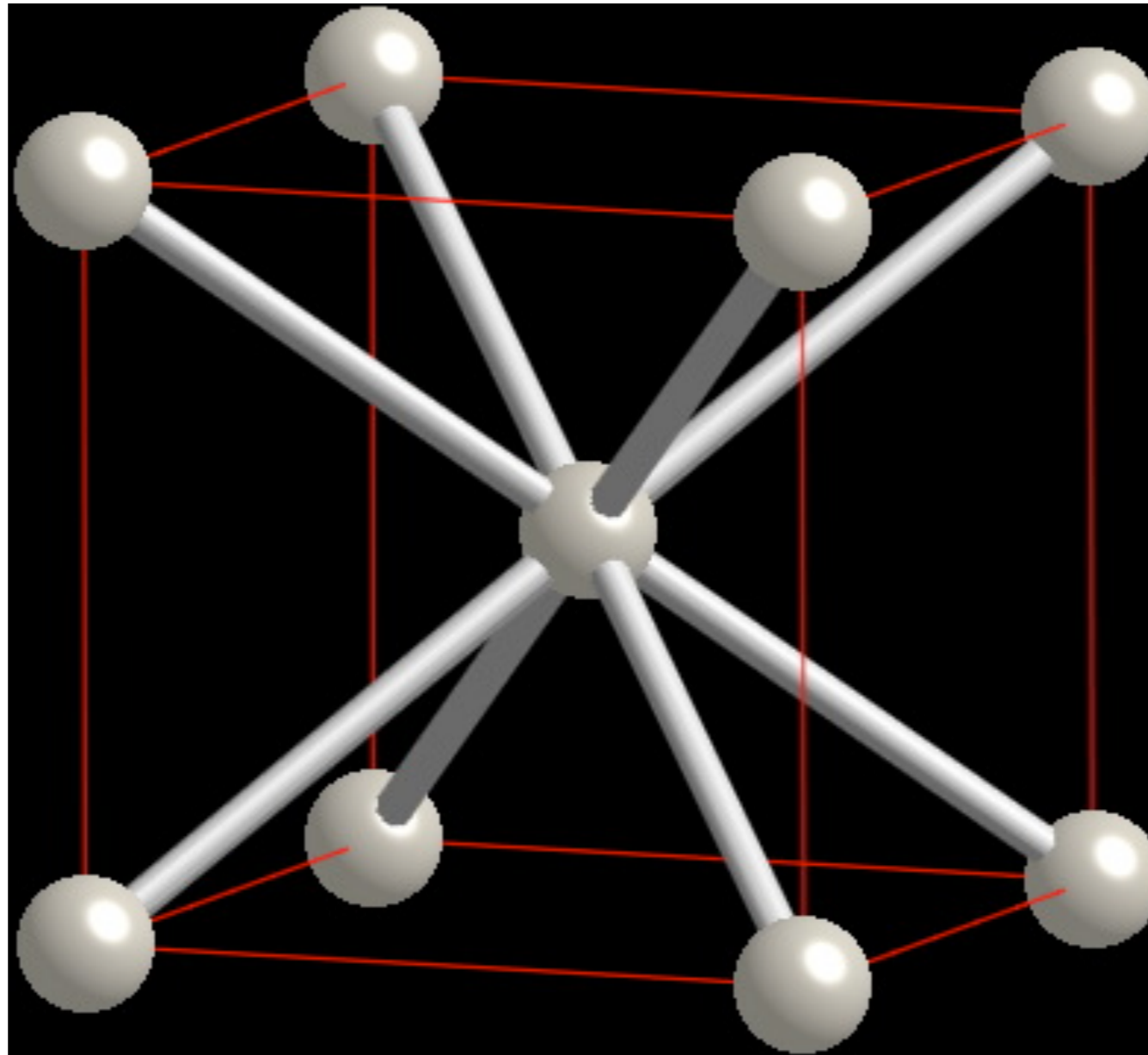
$AB \rightarrow \delta B + A\delta$ (111) plane

$AB \rightarrow \gamma B + A\gamma$ ($\bar{1}\bar{1}\bar{1}$) plane

$|hkl\rangle$ "points" in positive direction

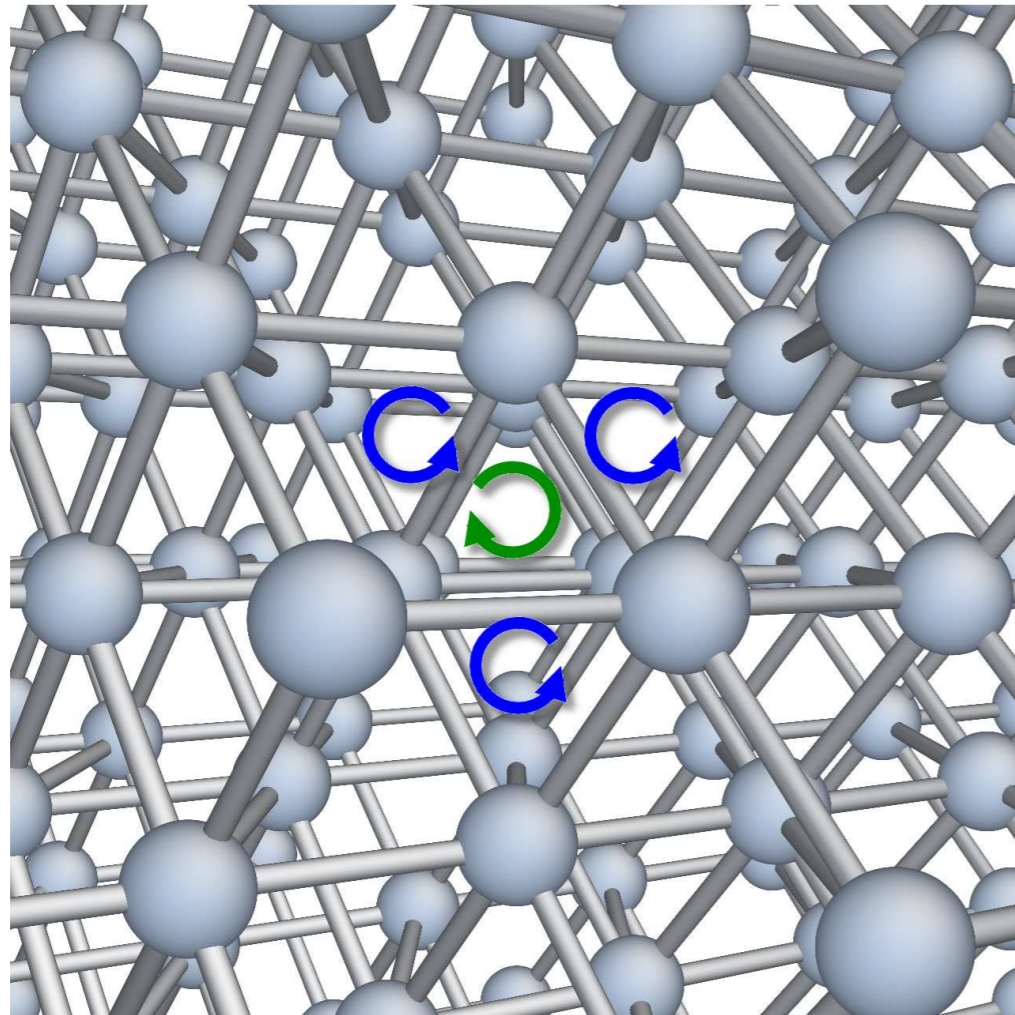


BCC crystal structure

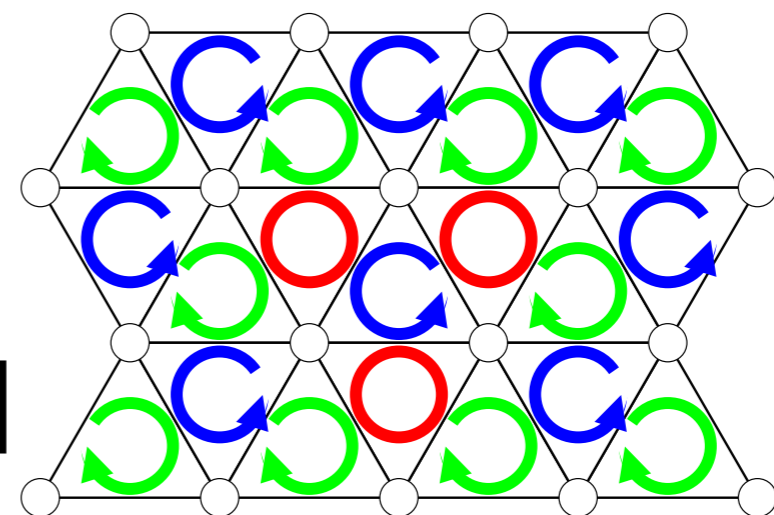
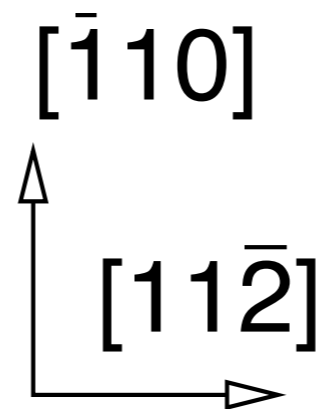
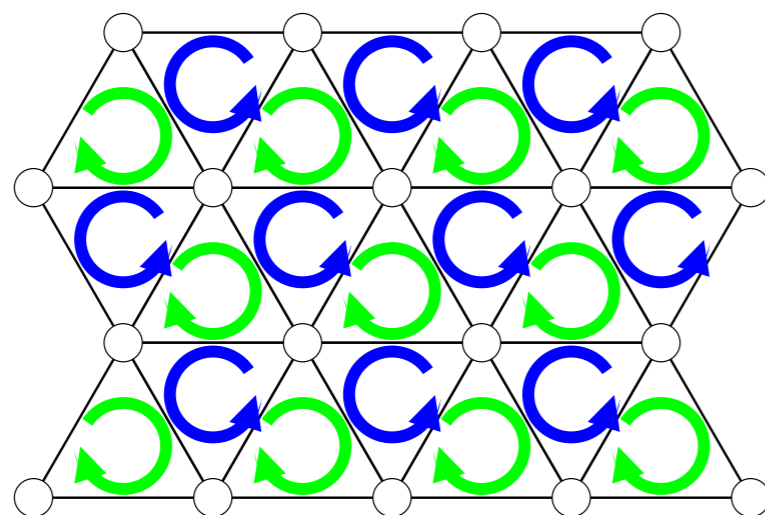
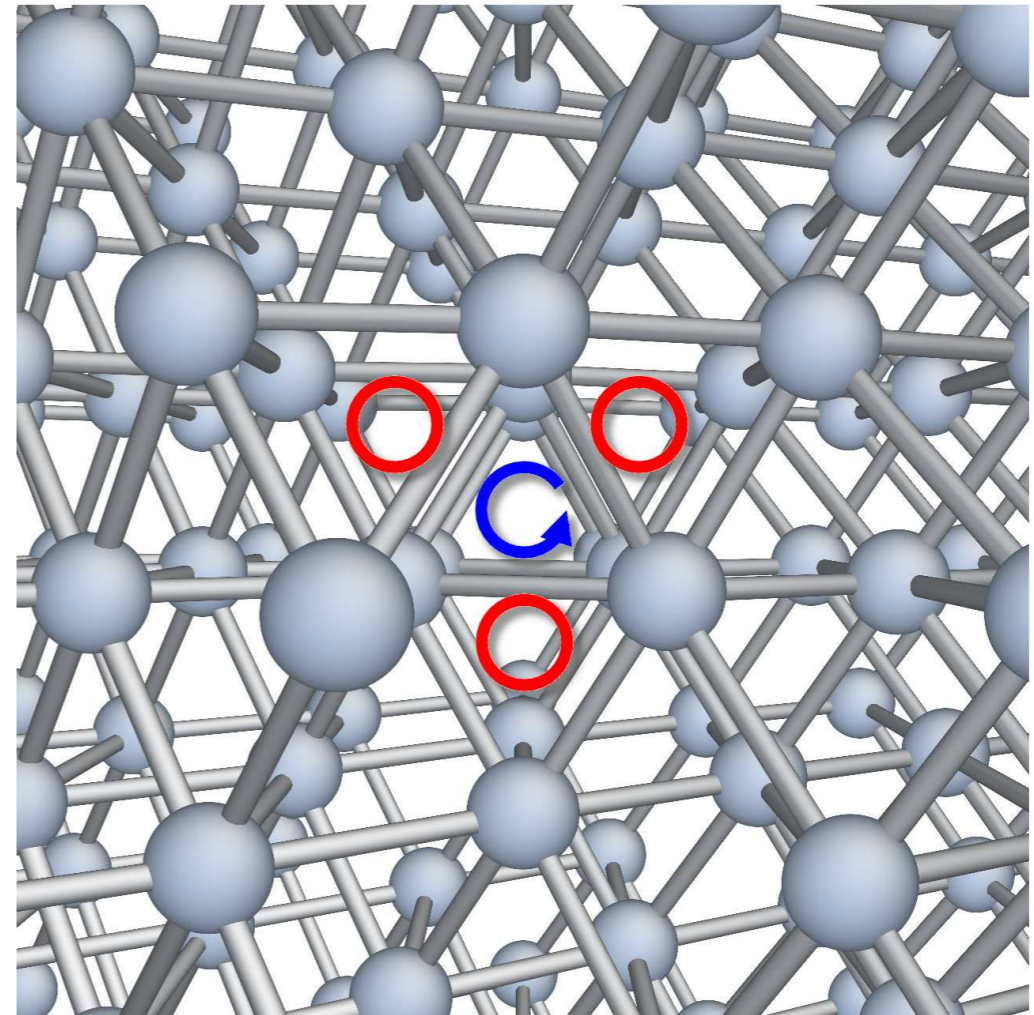


BCC [111] screw dislocation

bulk bcc

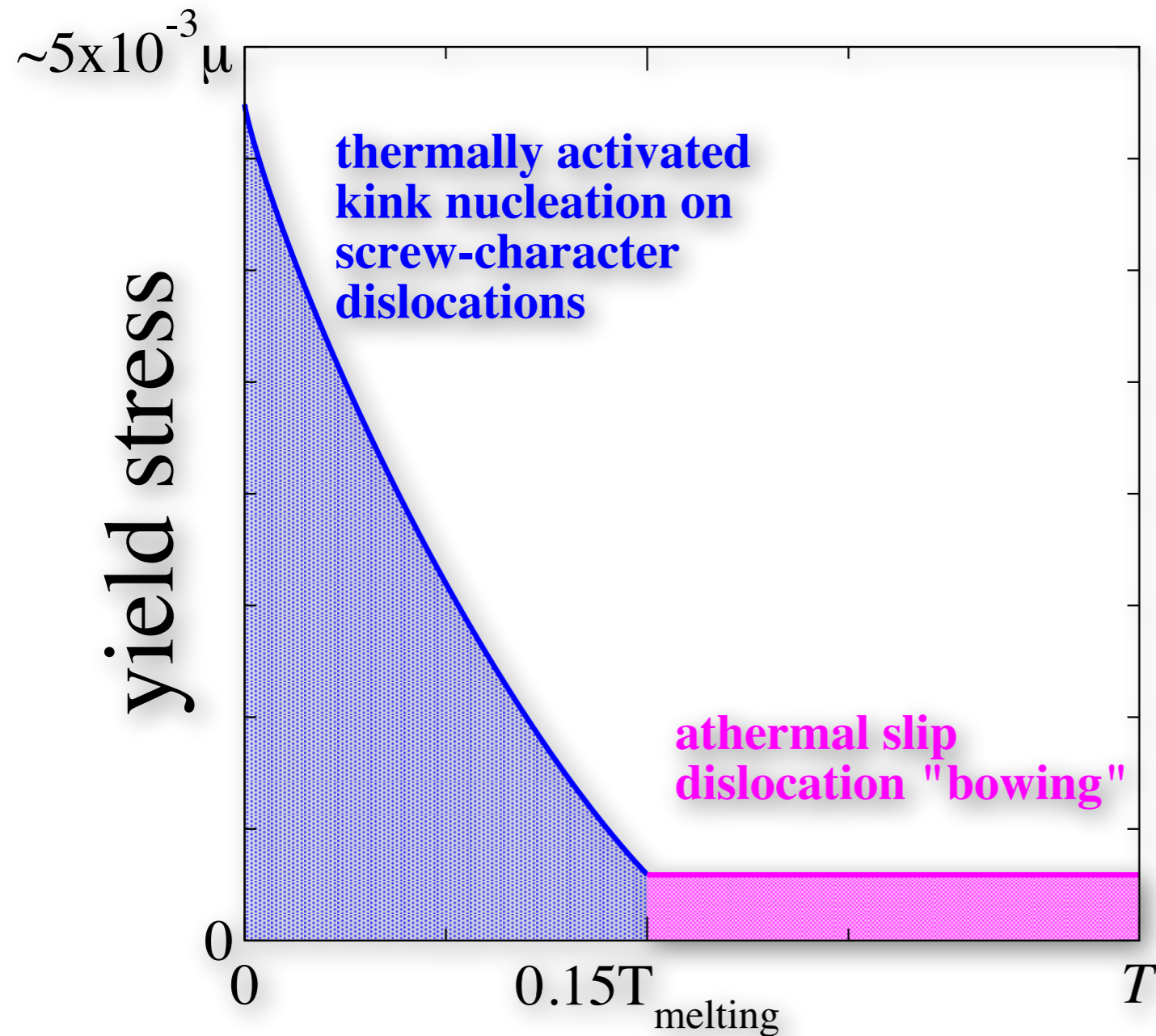


bcc screw dislocation

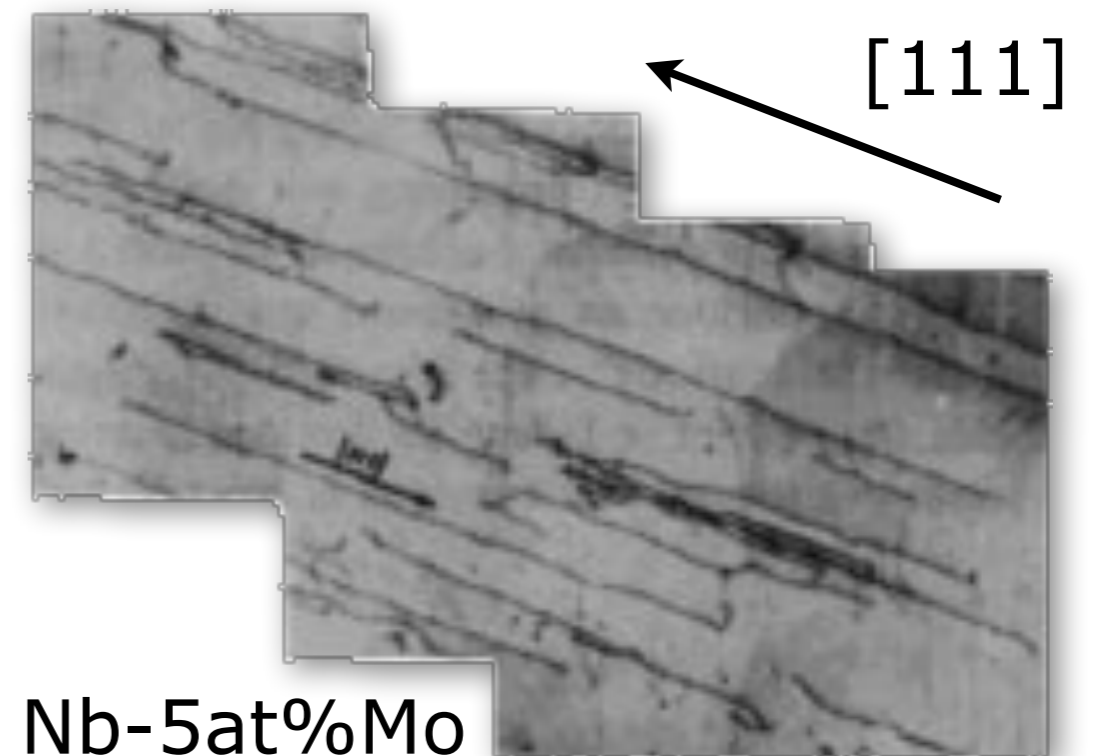


BCC plastic deformation

- Below 15% of melting T , strongly temperature dependent
- Often poor low-temperature ductility—related to high strength
- Non-Schmid effects: tension/compression asymmetry
- Controlled by $[111]$ screw-character dislocations

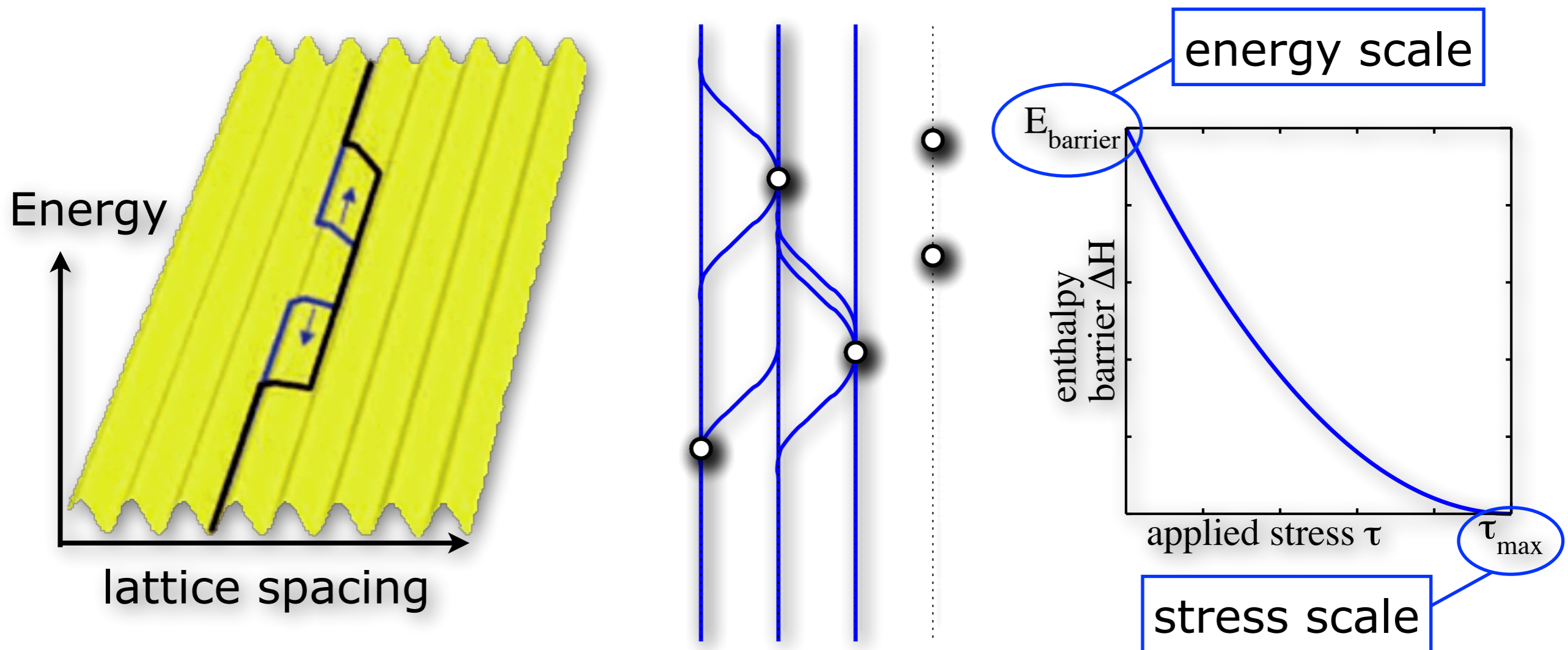


Classical theory (Hirsch) interpreted behavior as due to non-planar dislocation cores: dislocation moves by creating "kinks" to next lattice site



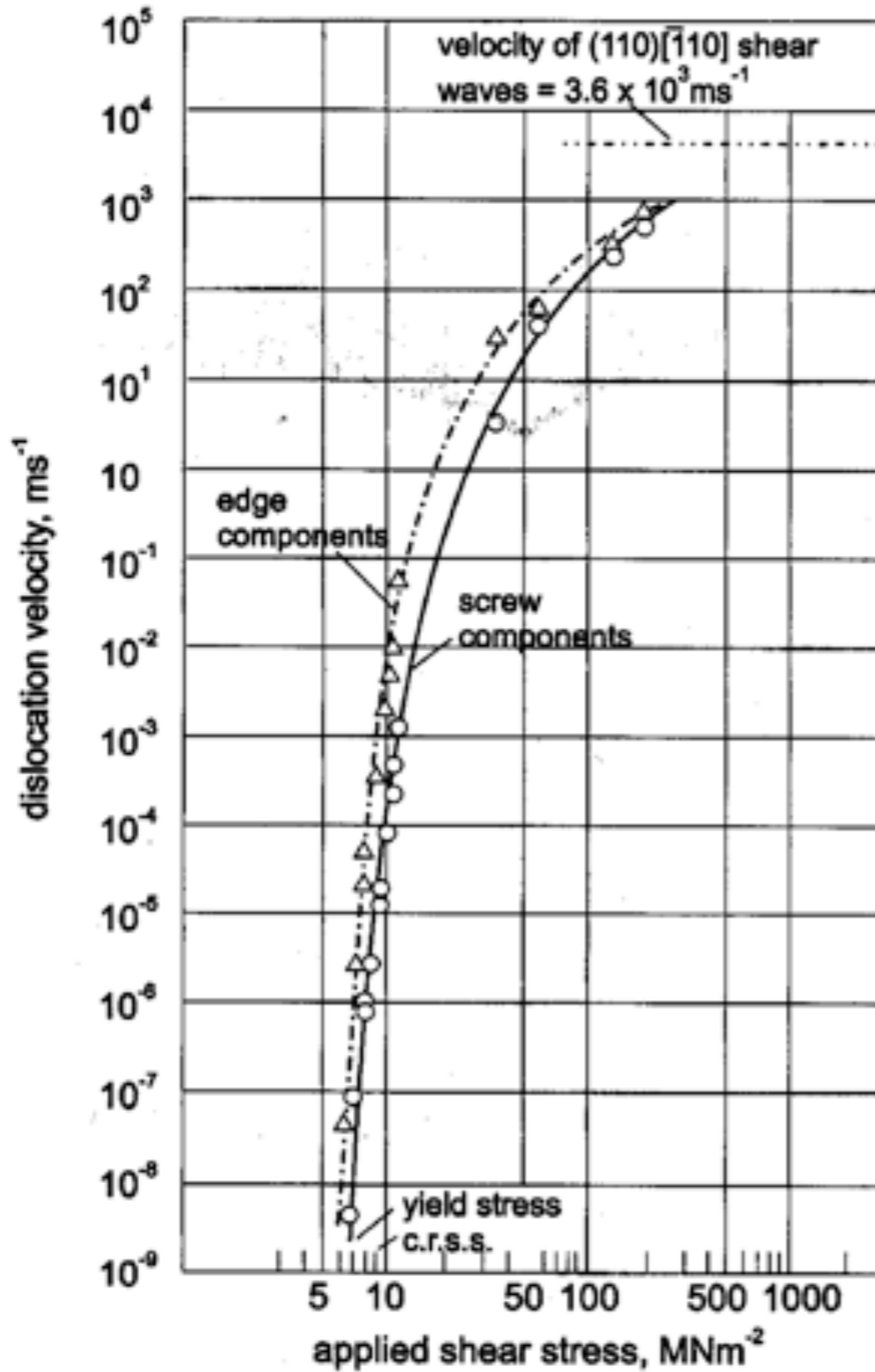
Thermally-activated slip (including solutes) 55

- Dislocation line from lattice site to site under applied stress
- Large Peierls stresses requires dislocation move via kinks
- Finite temperatures overcome enthalpy barriers for
 1. double-kink nucleation (both at and away from solutes)
 2. kink migration past solutes



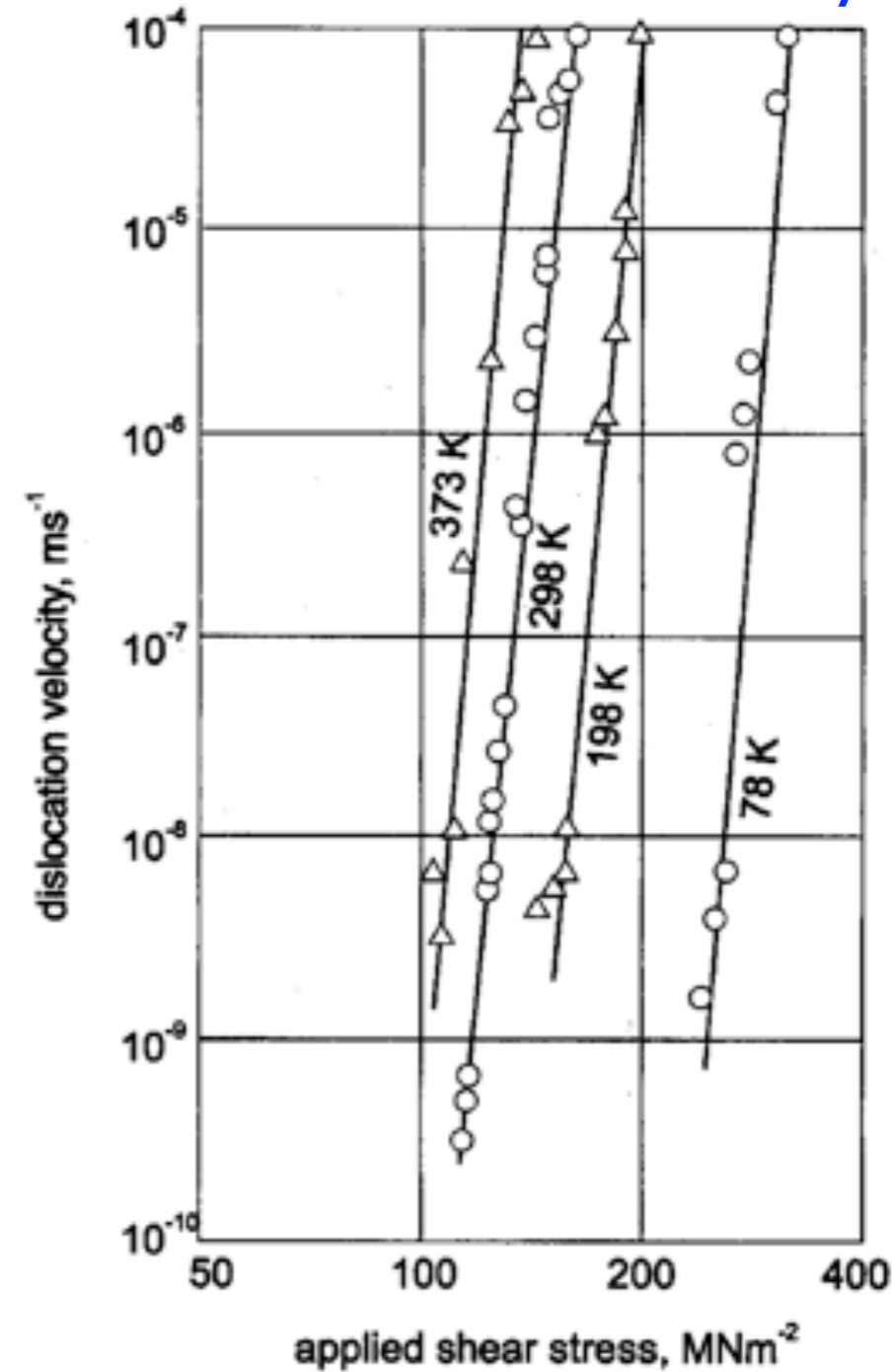
Applied stress reduces enthalpy barriers for both processes

LiF
crystal



(a)

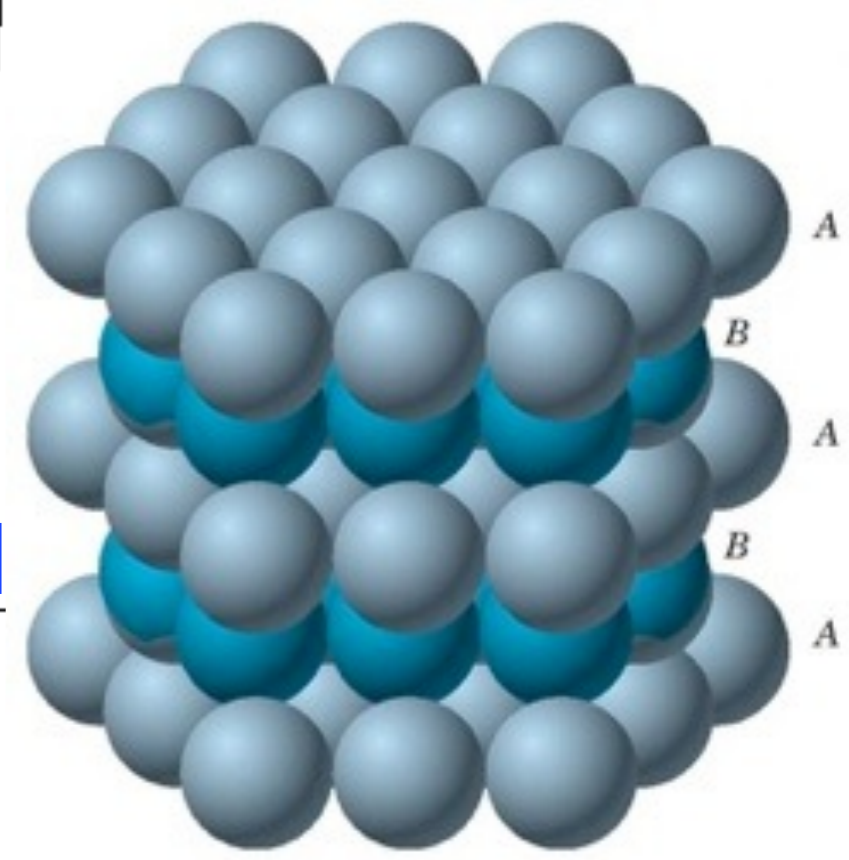
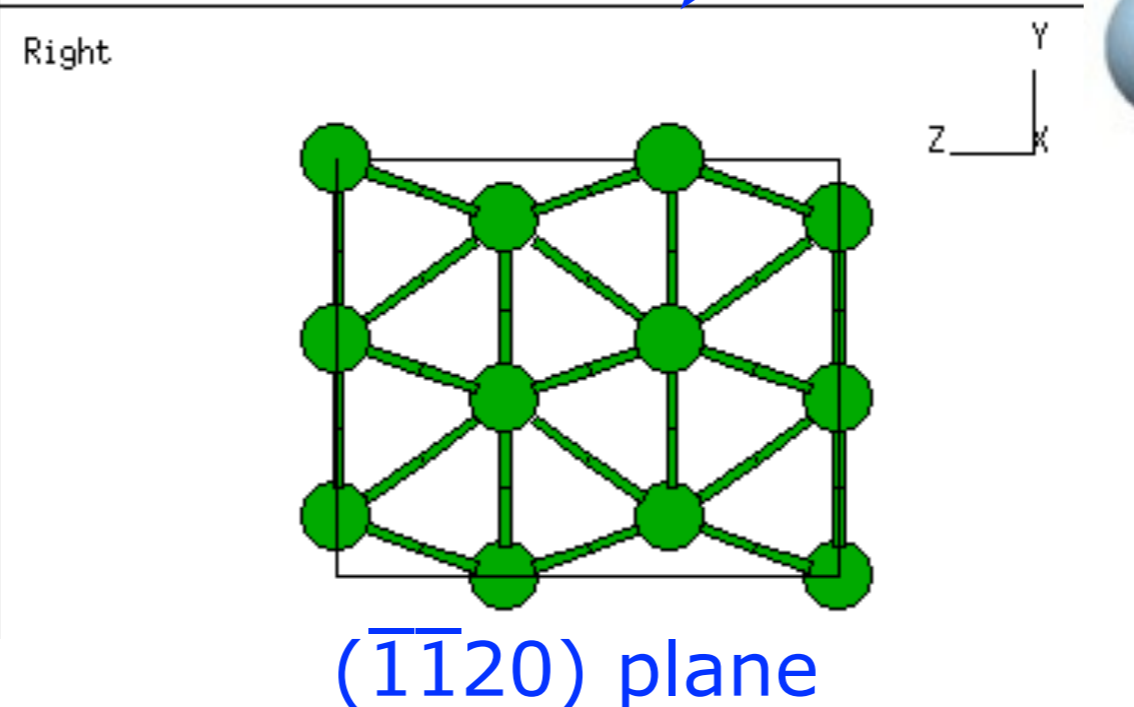
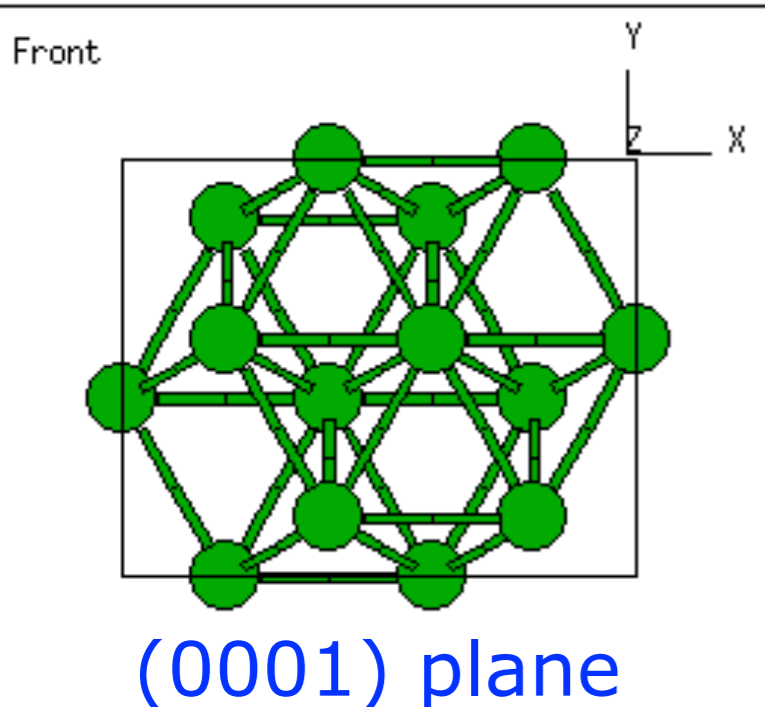
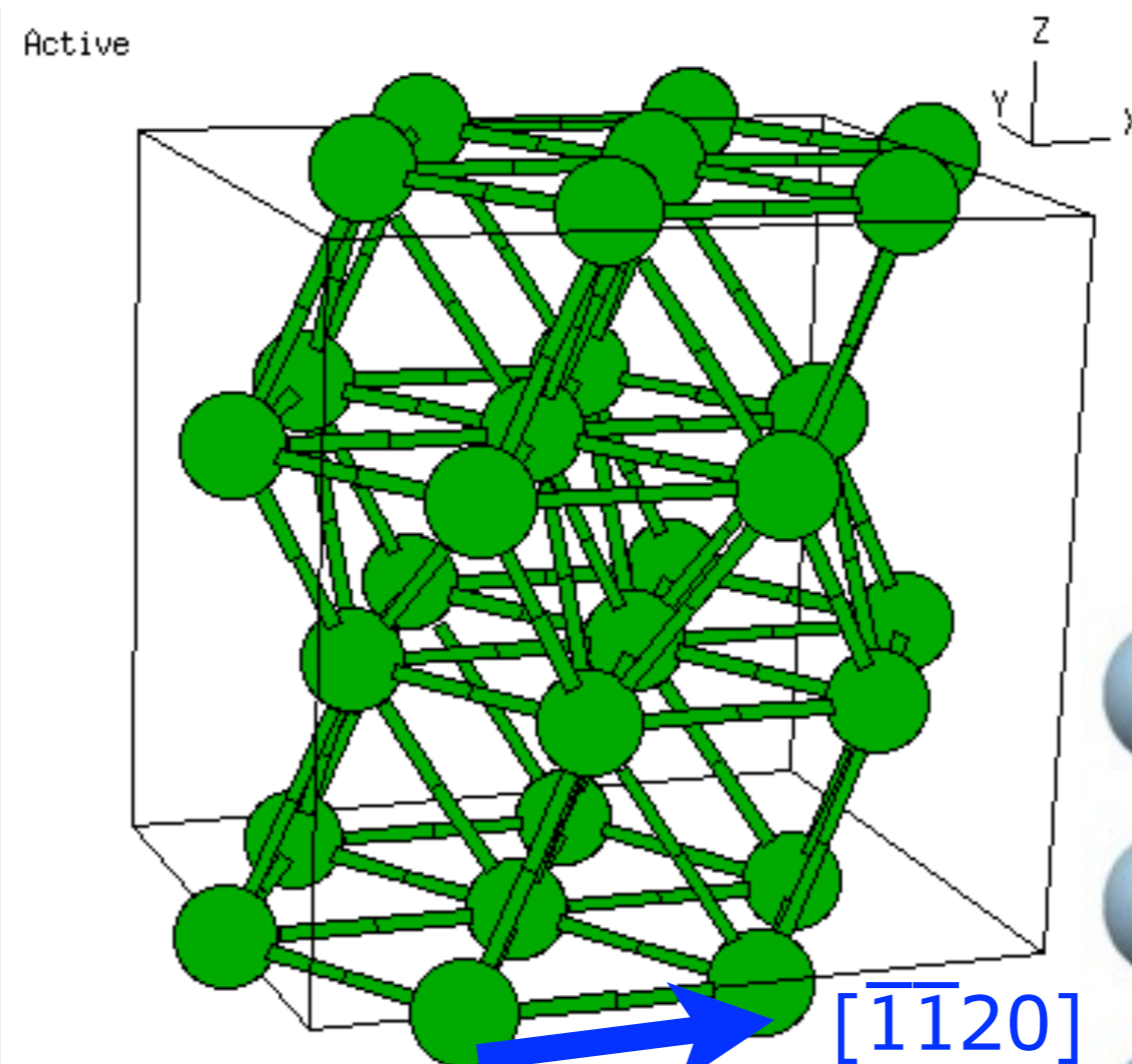
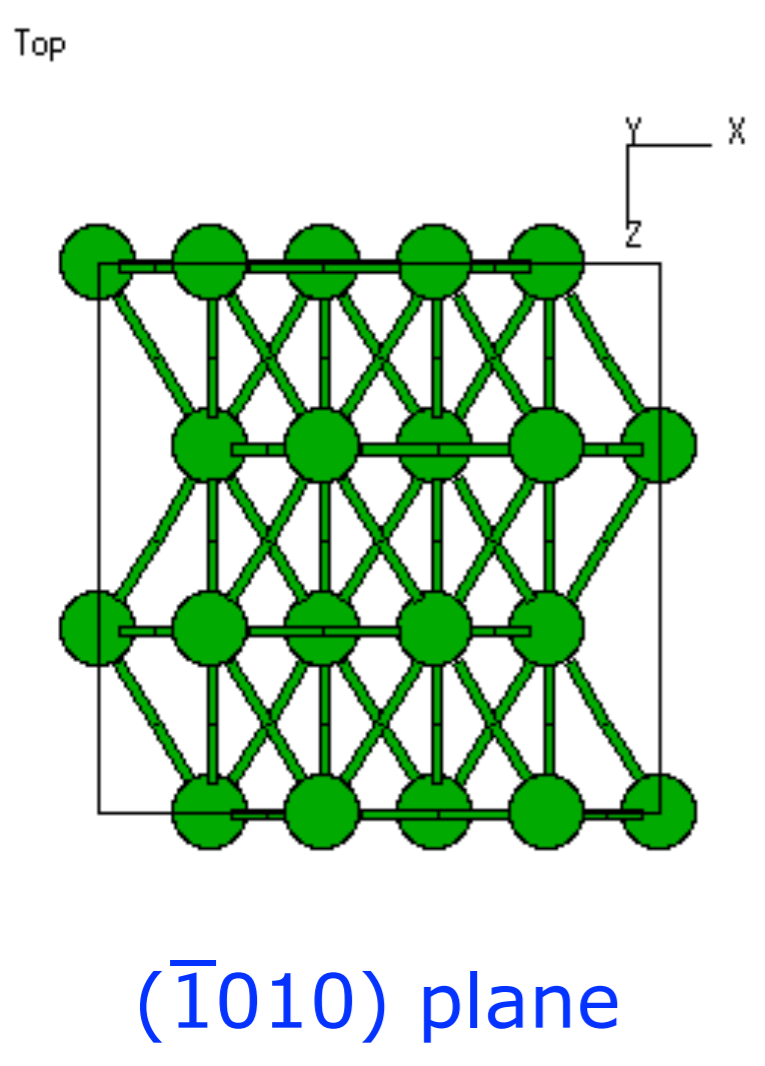
Fe-3.25%Si
crystal



(b)

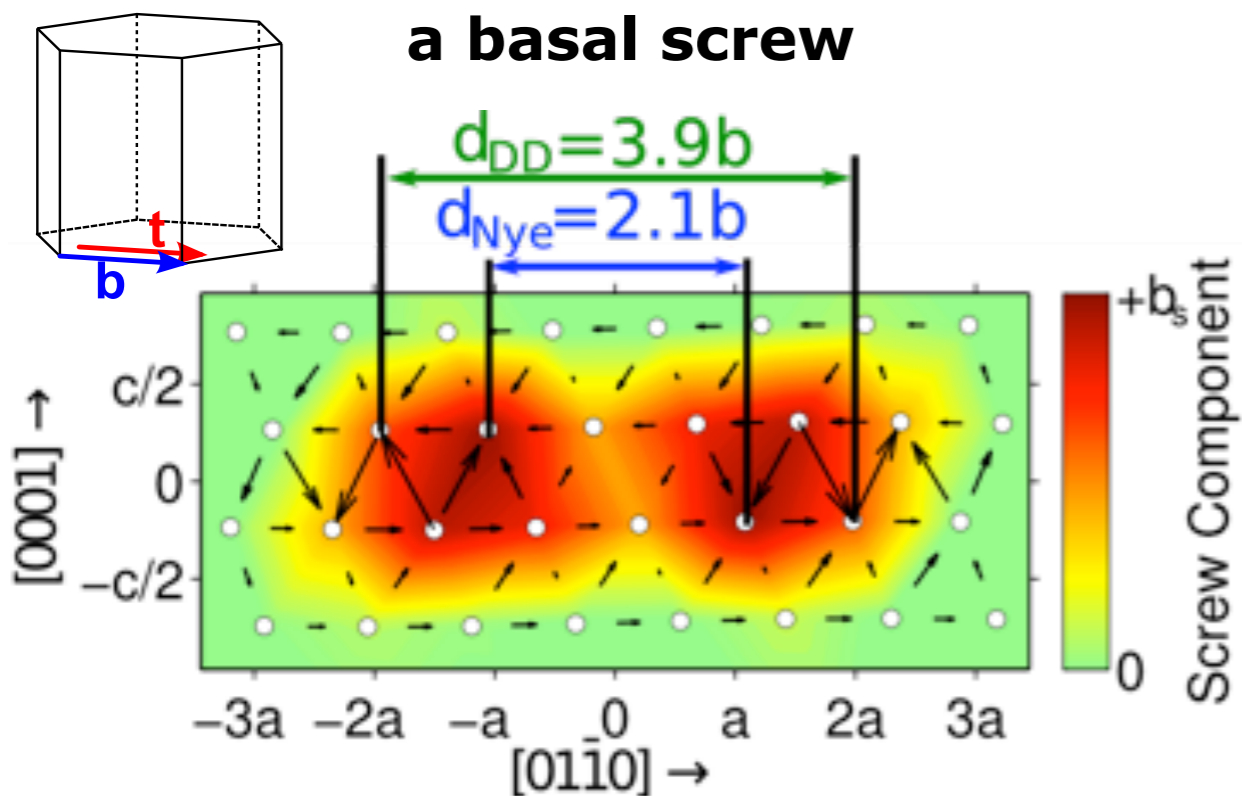
Figure 3.11 (a) Stress dependence of the velocity of edge and screw dislocations in lithium fluoride. (From Johnston and Gilman, *J. Appl. Phys.* **30**, 129, 1959.) (b) Stress dependence of the velocity of edge dislocations in 3.25 per cent silicon iron at four temperatures. (After Stein and Low, *J. Appl. Phys.* **31**, 362, 1960.)

HCP crystal structure

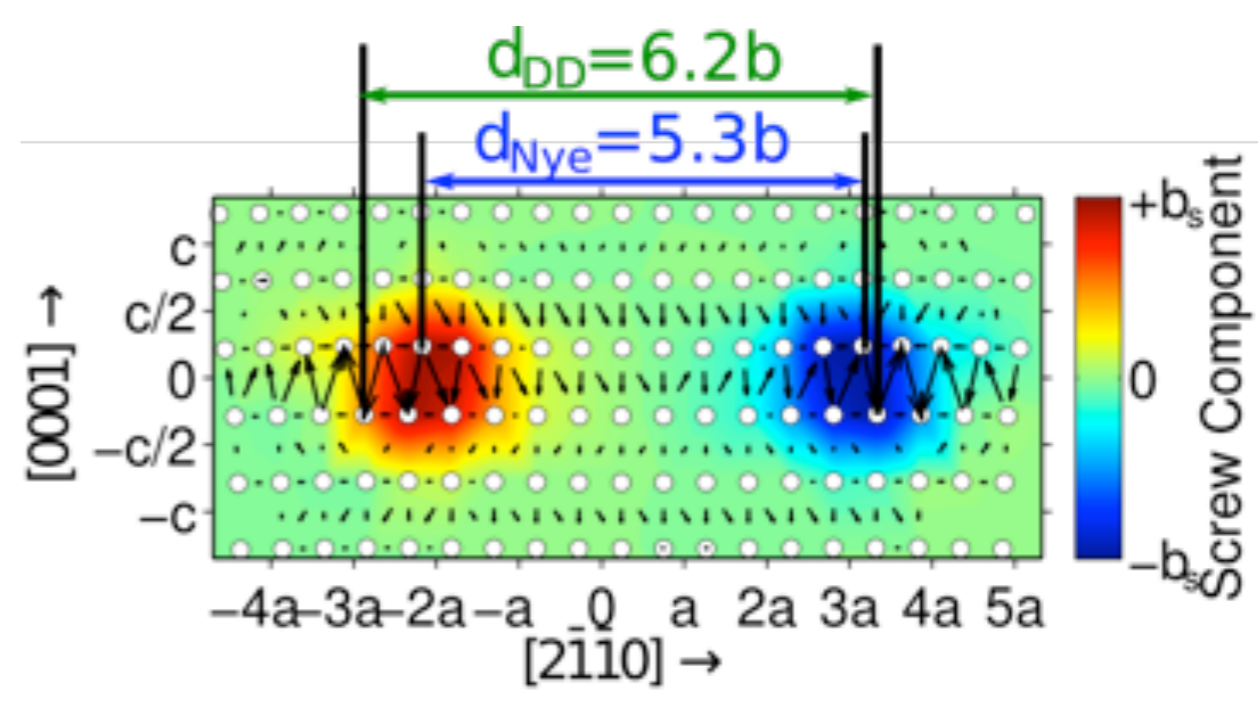
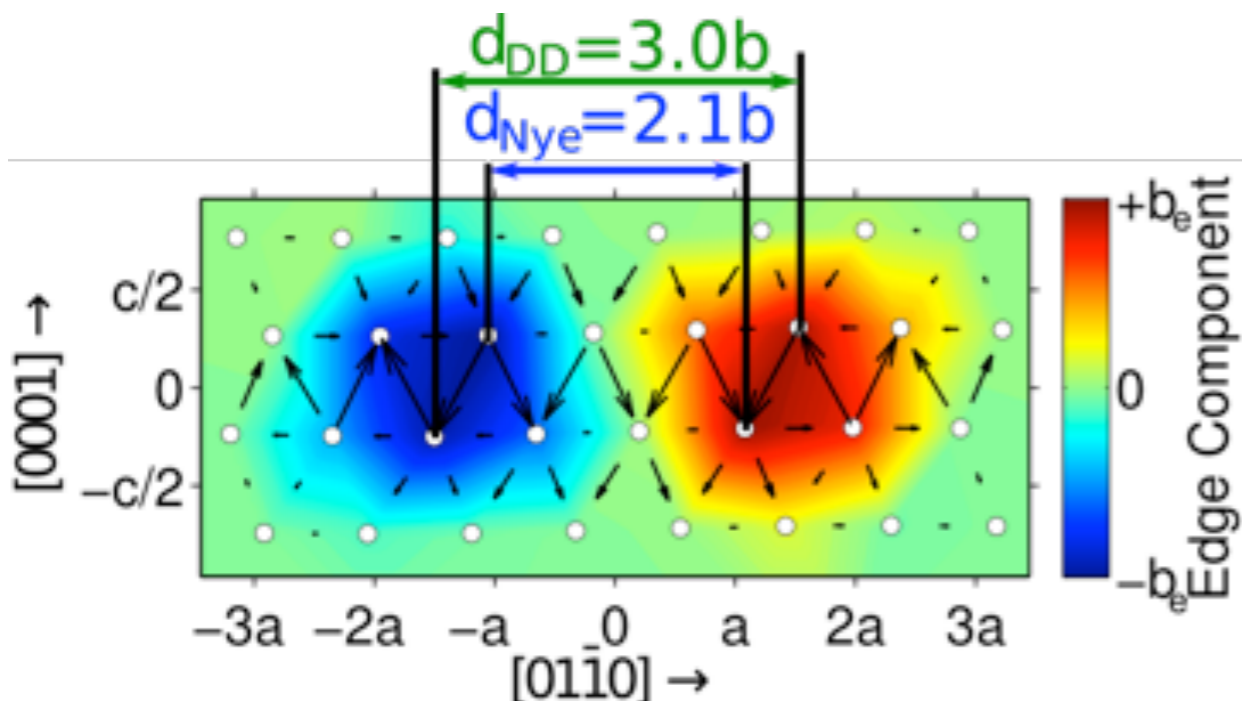
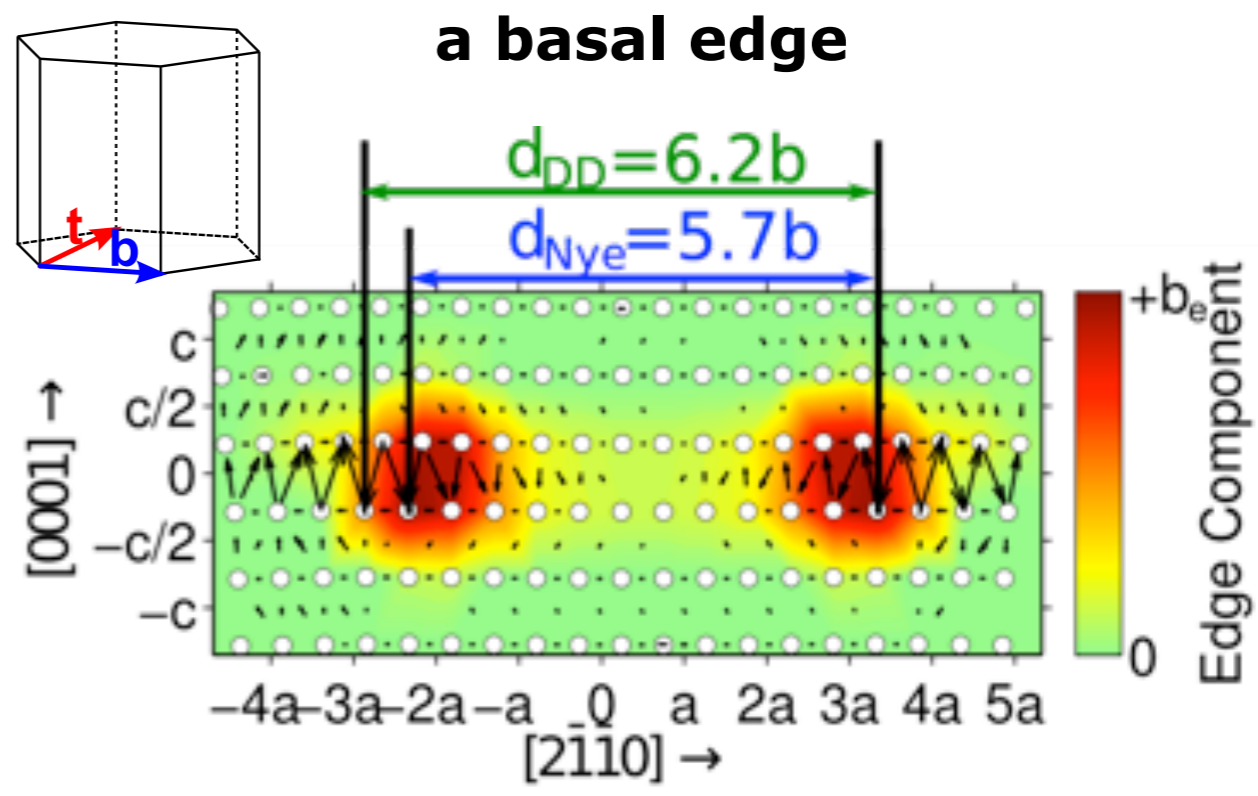


Mg dislocation cores: a-type basal

a basal screw

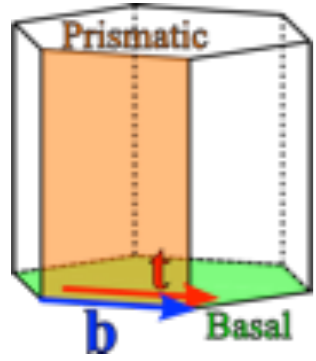


a basal edge



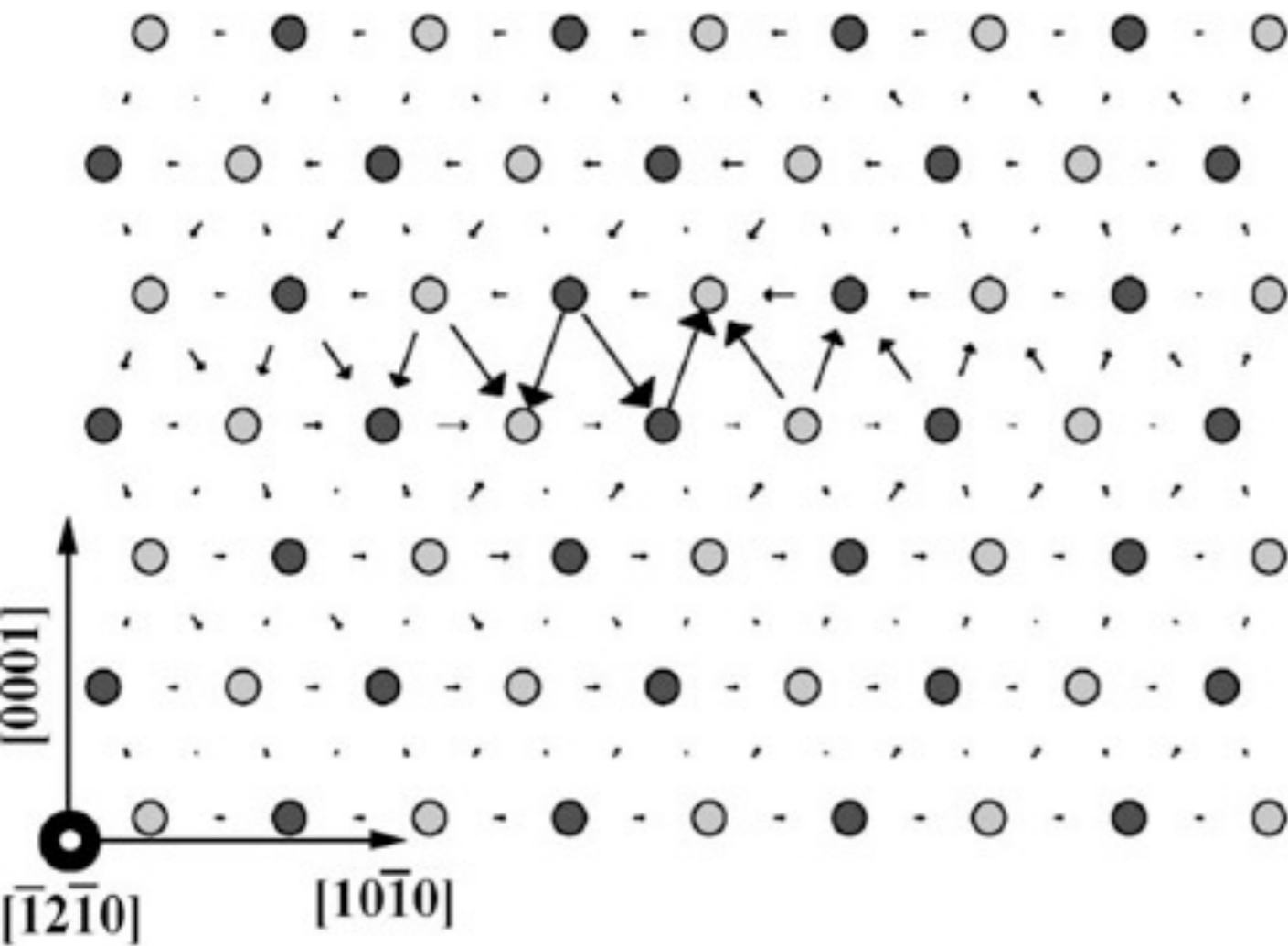
c.f.: elasticity (34 mJ/m^2) = $3.7b$

c.f.: elasticity (34 mJ/m^2) = $7.3b$

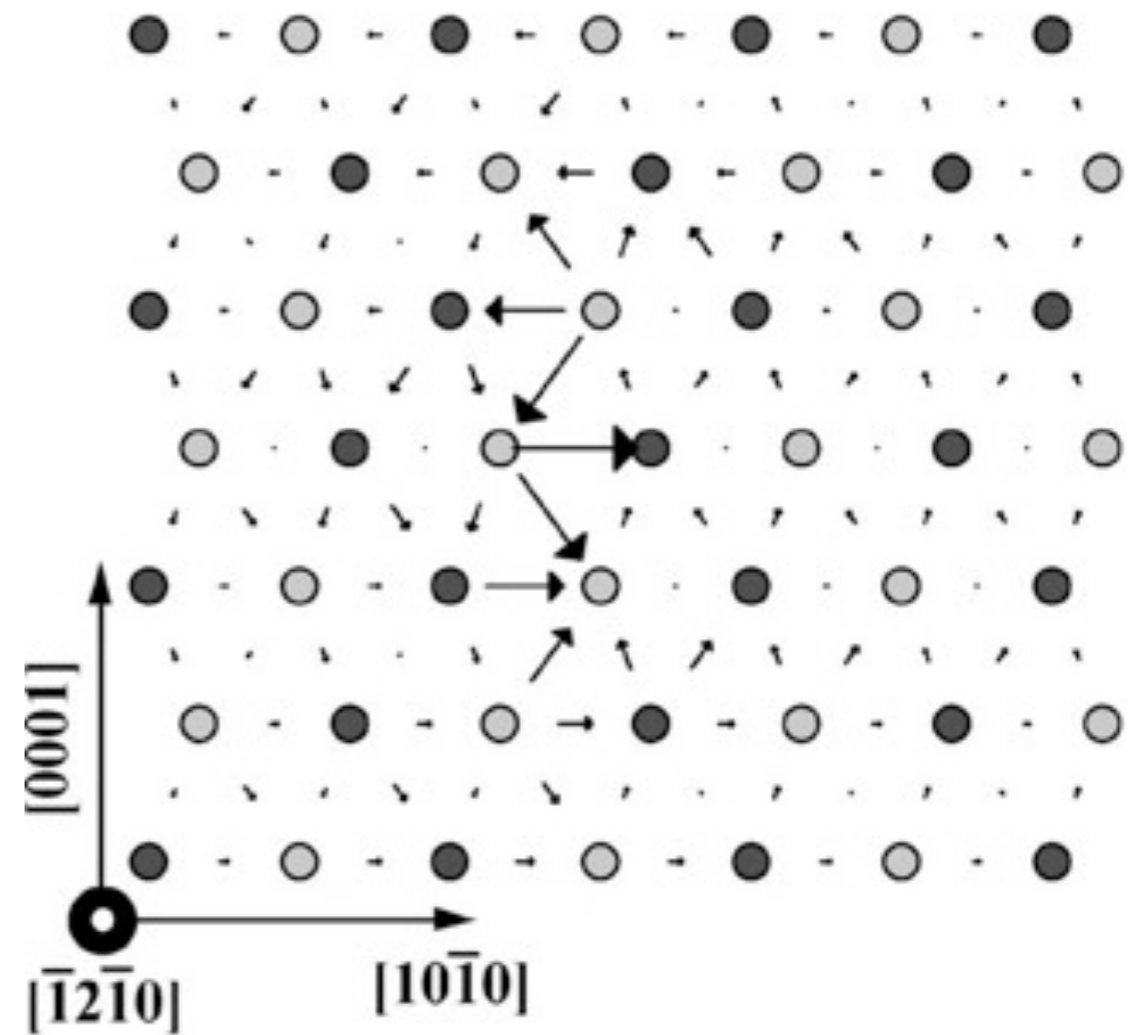


Basal and prismatic dislocation cores: Ti 59

Basal a-type screw dislocation

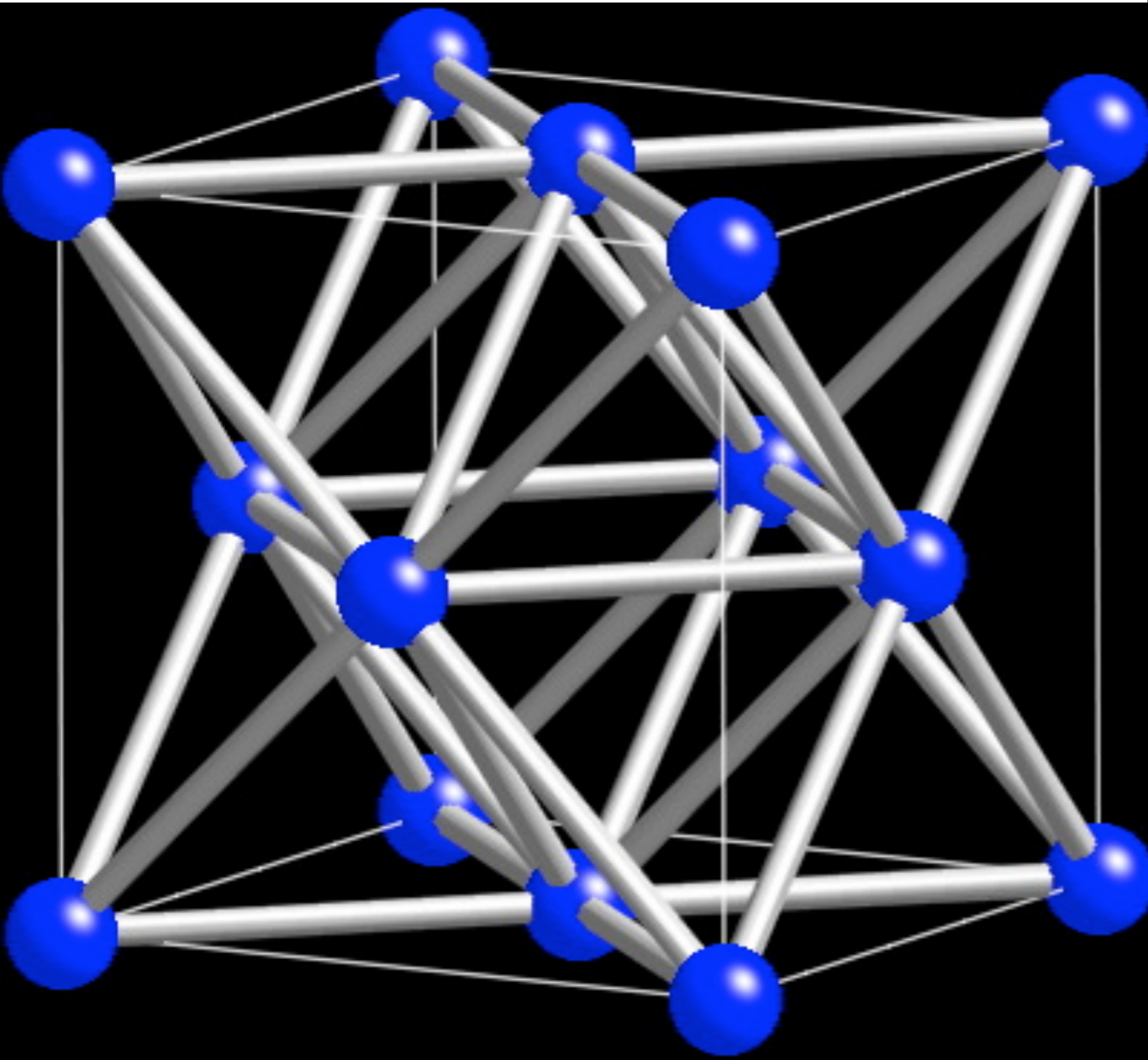


Prismatic a-type screw dislocation

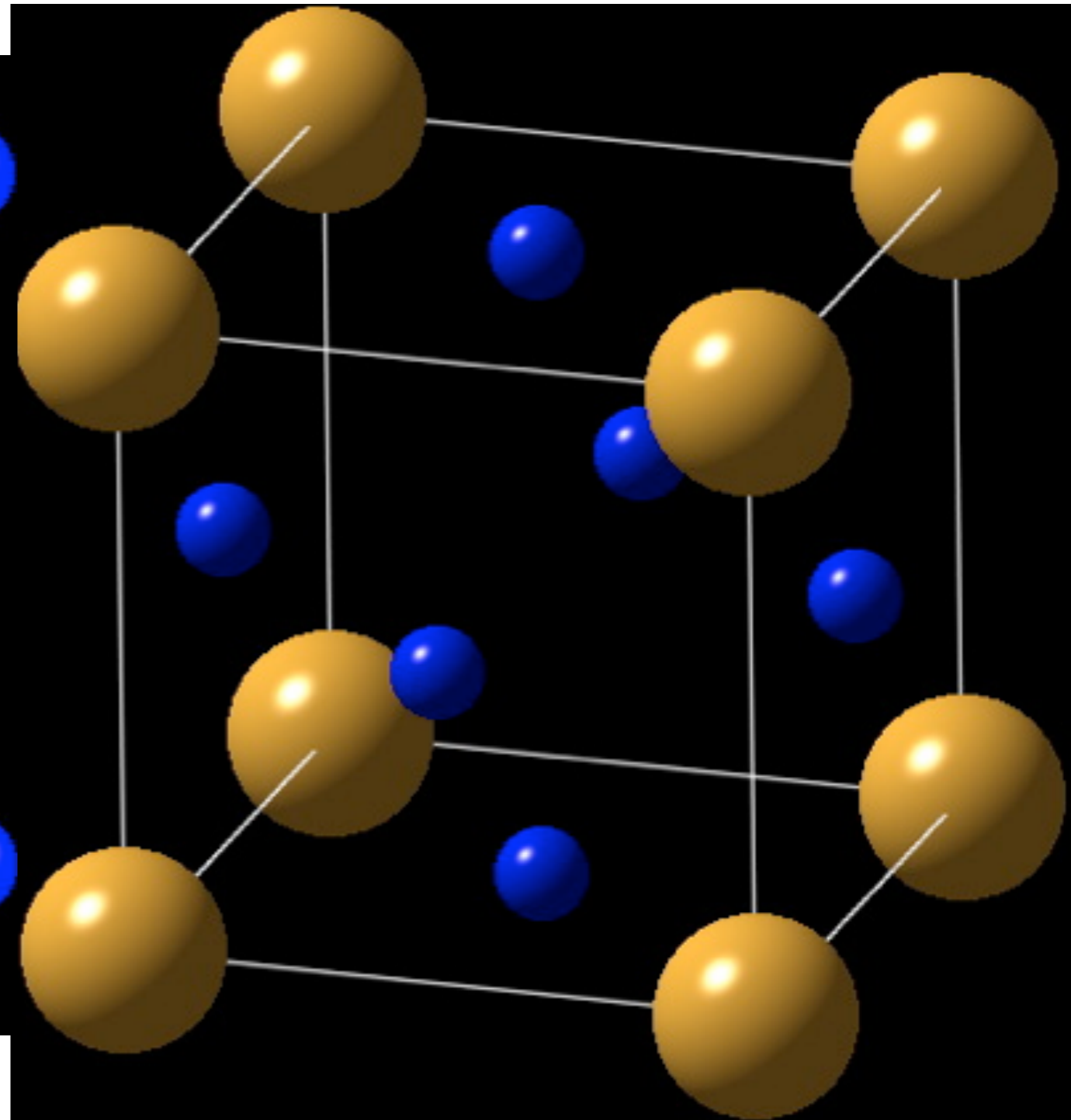


L1₂ (based on FCC) crystal structure

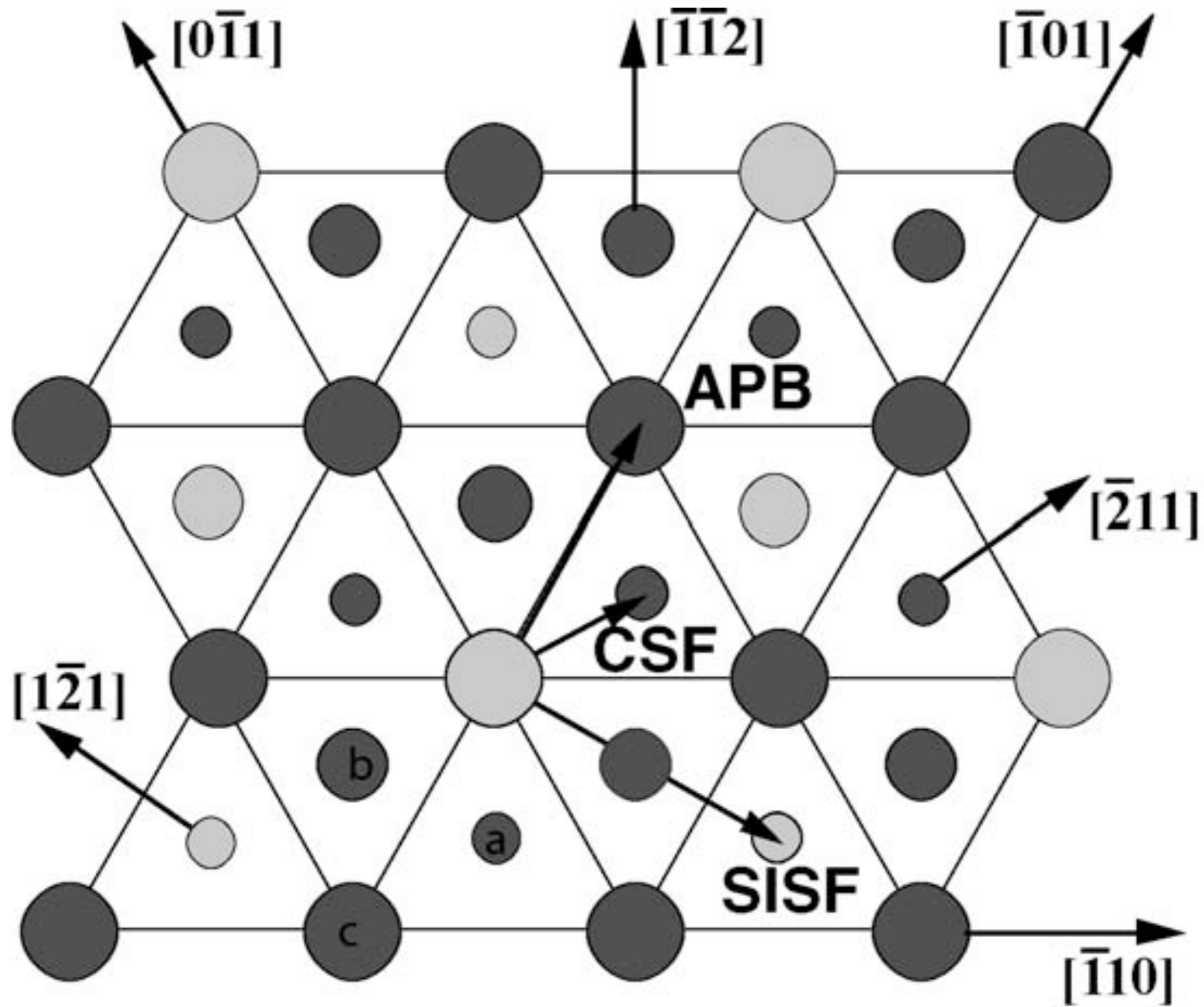
Ni



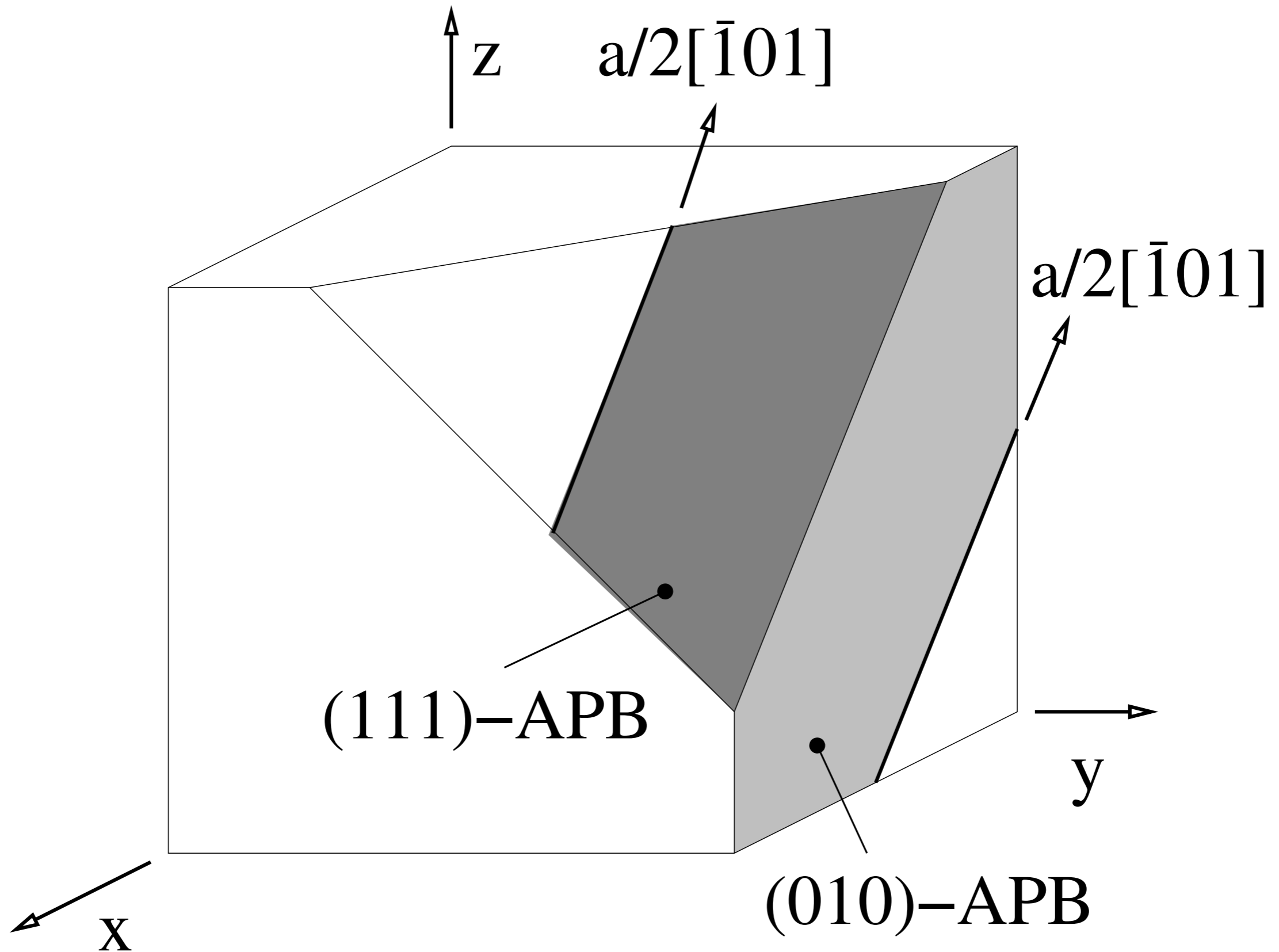
Ni₃Al



$L1_2$ (111) stacking fault



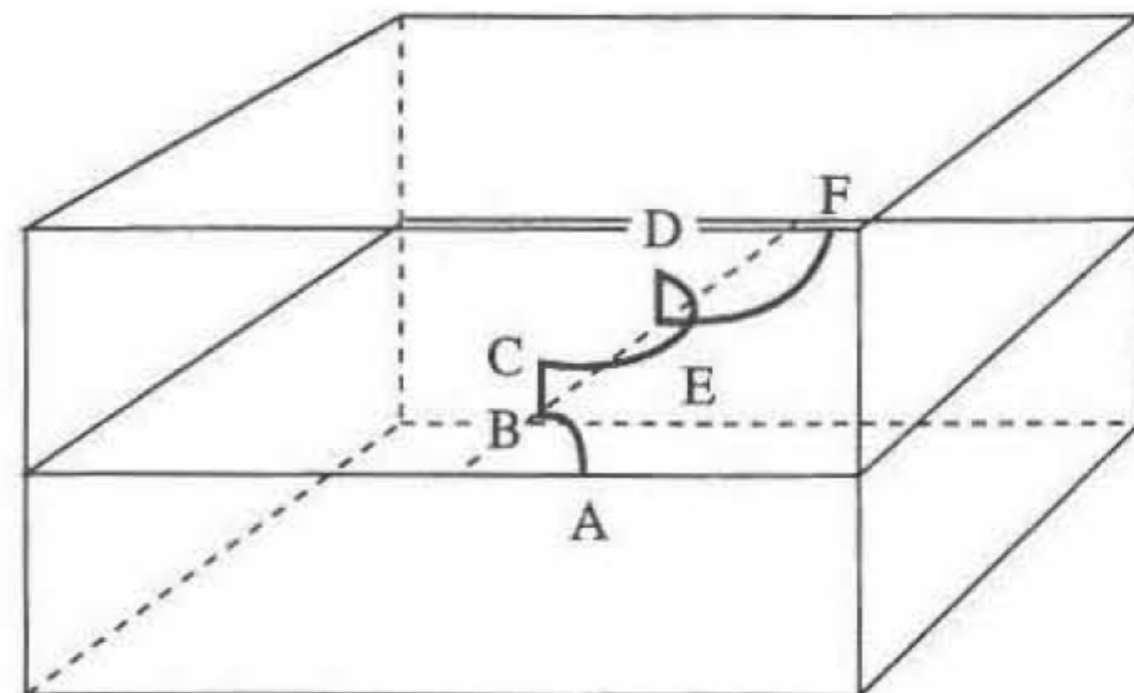
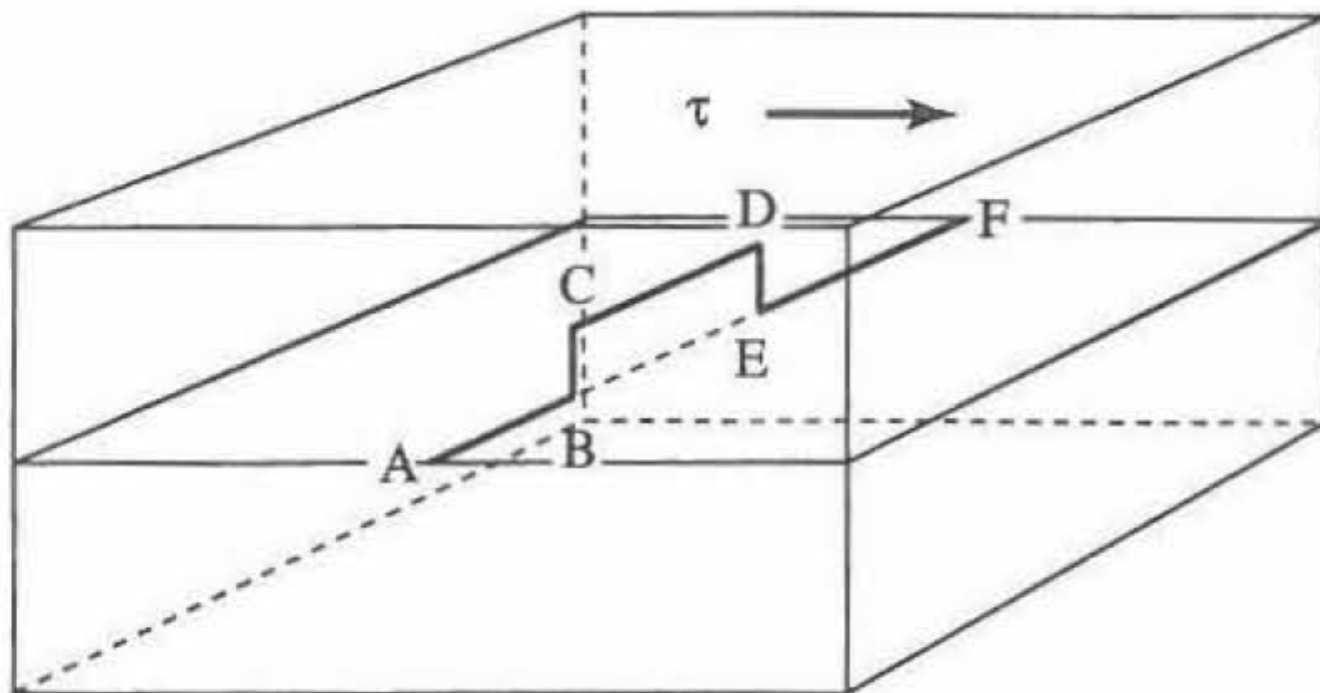
L1₂ Kear-Wilksdorf lock



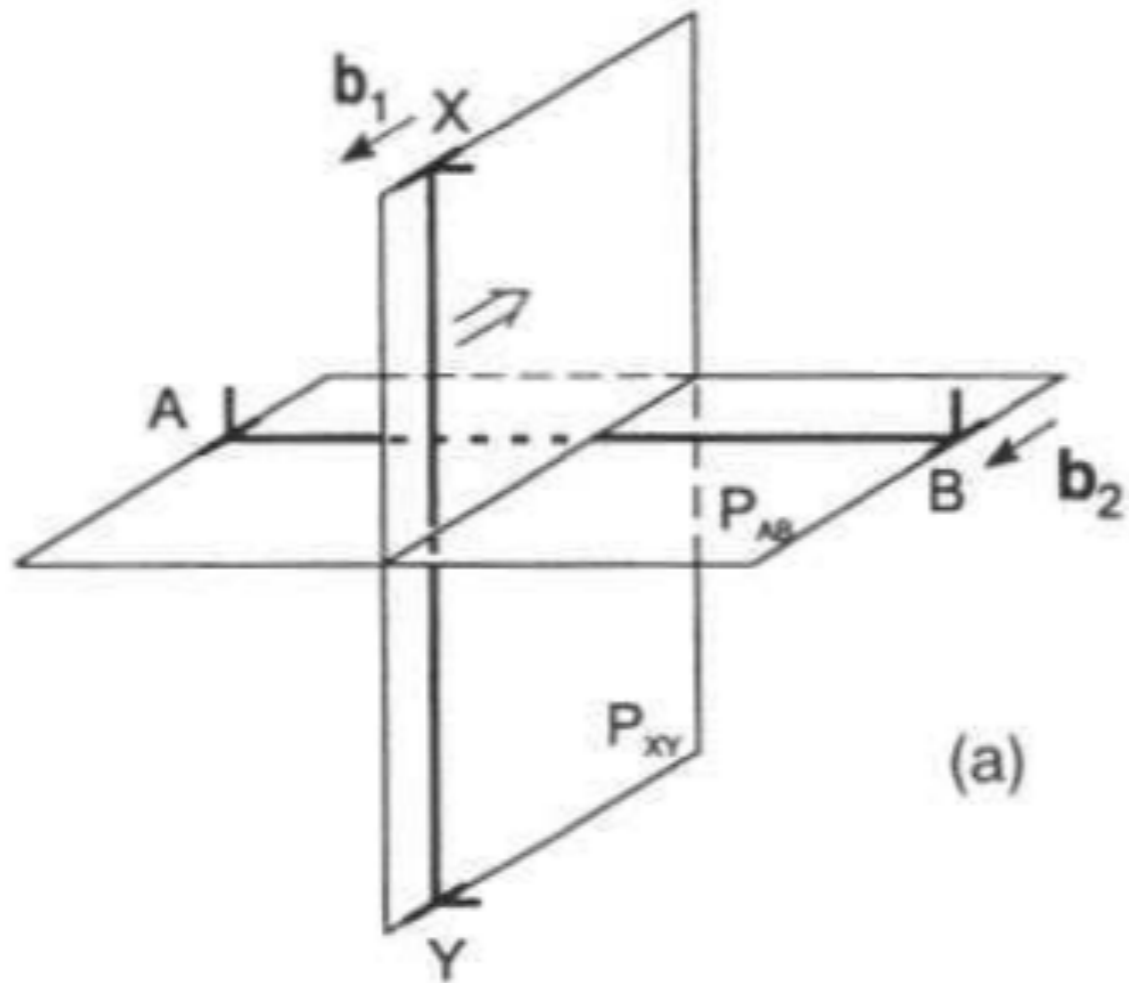
Dislocation/dislocation interactions

63

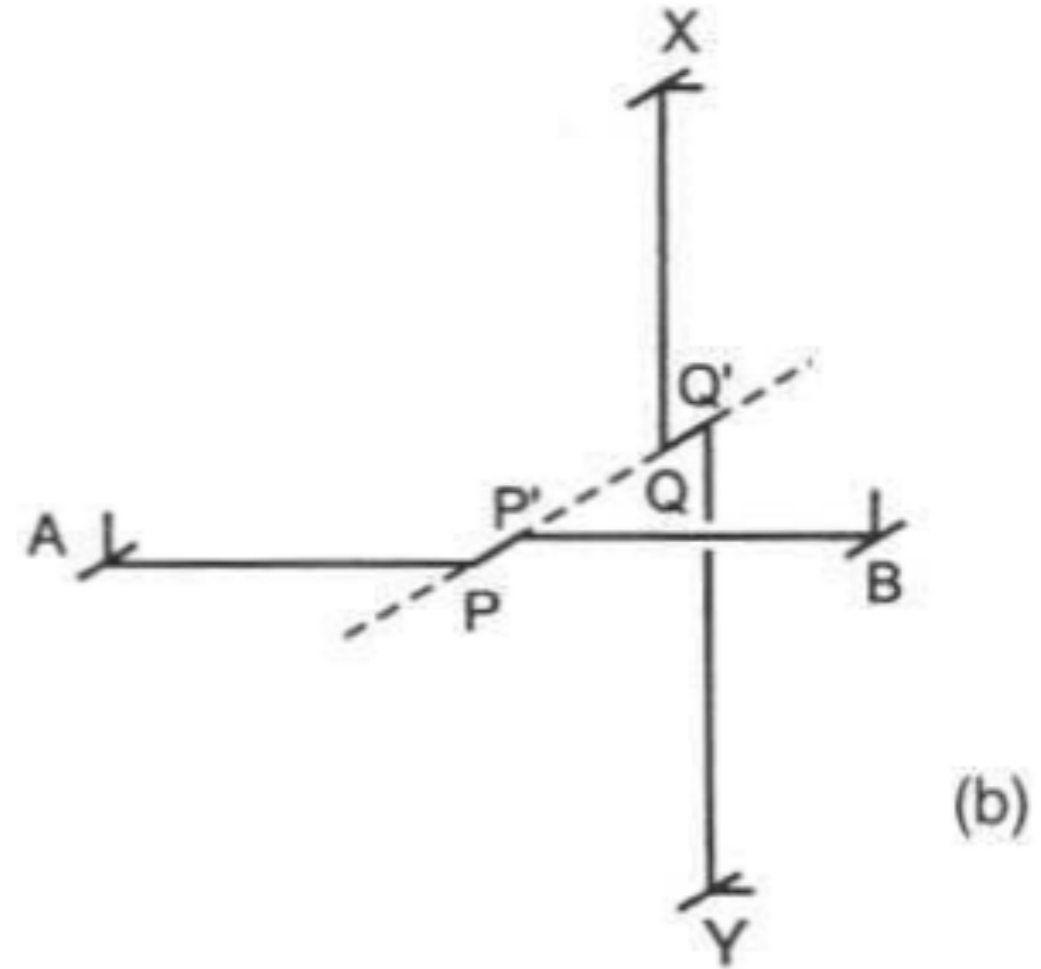
- We've already encountered two:
 - Stress + Peach-Koehler force (long-range) interaction
 - Dislocation reaction: two dislocations combining into a third
- Third type of dislocation/dislocation interaction: jogs
 - A dislocation passes through another dislocation, each leaves behind a "step" in the other dislocation corresponding to the Burgers vector.
 - If the step is **in the slip plane**, it is a **kink** (kinks are usually mobile)
 - If the step is **out of the slip plane**, it is a **jog** (jogs are immobile)
 - Jogs will usually pin a dislocation line to that point in space



Edge / edge dislocation intersection

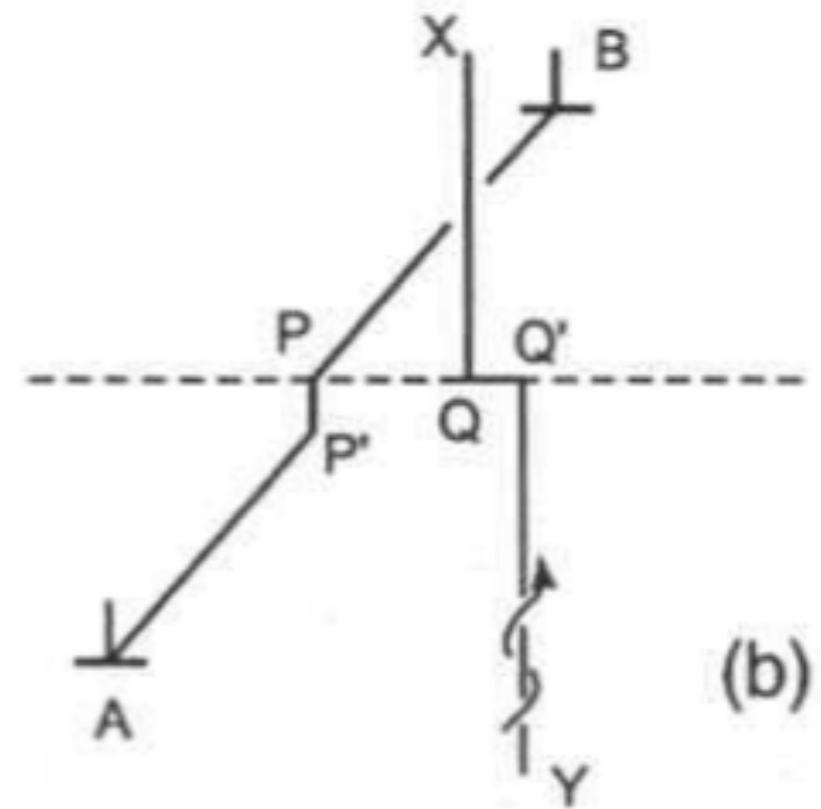
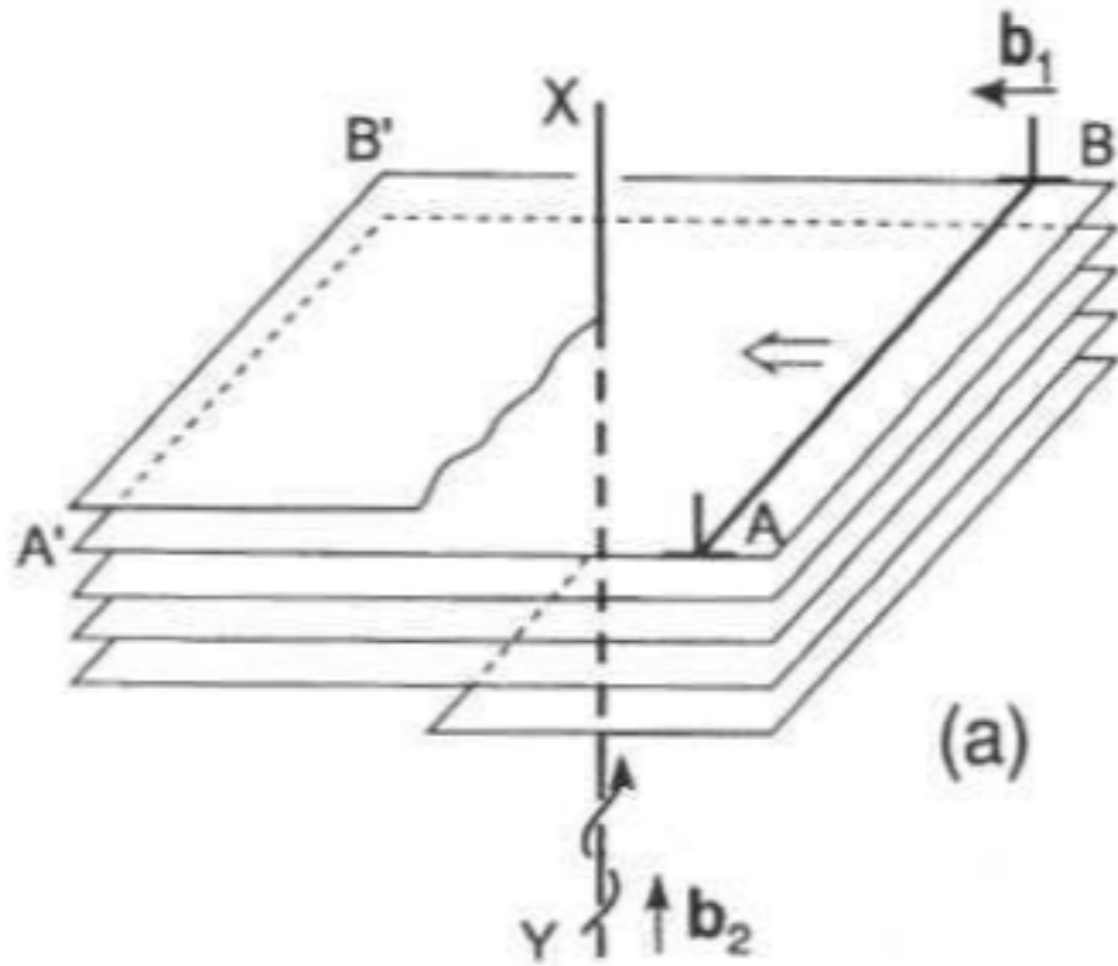


(a)

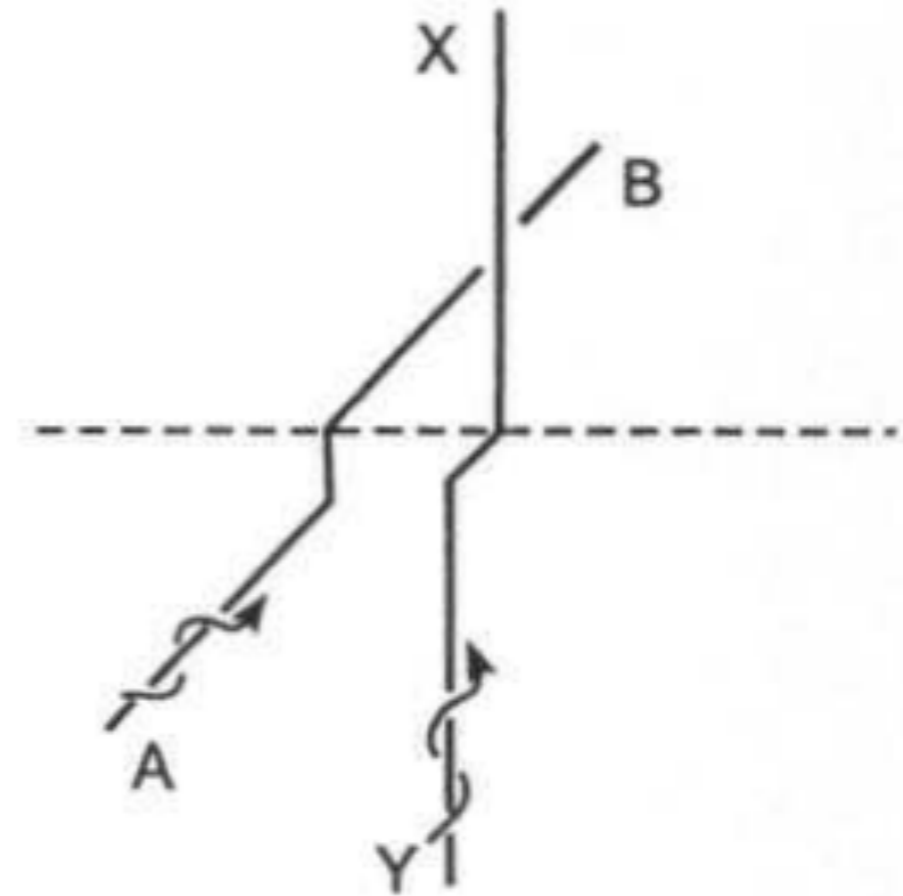
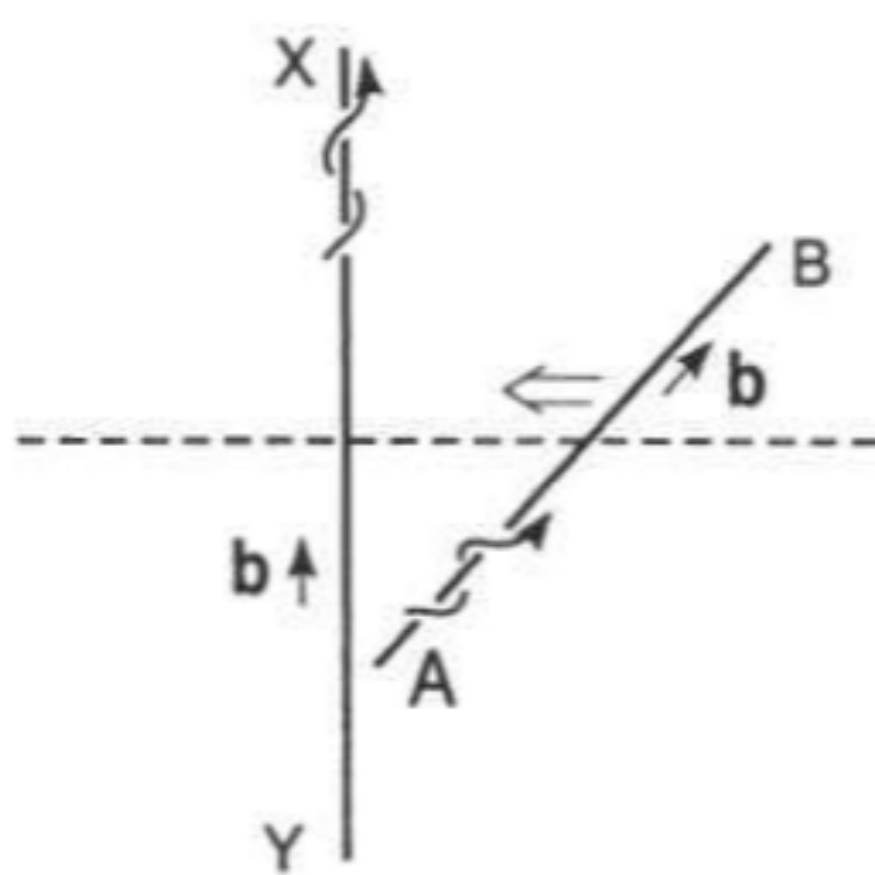


(b)

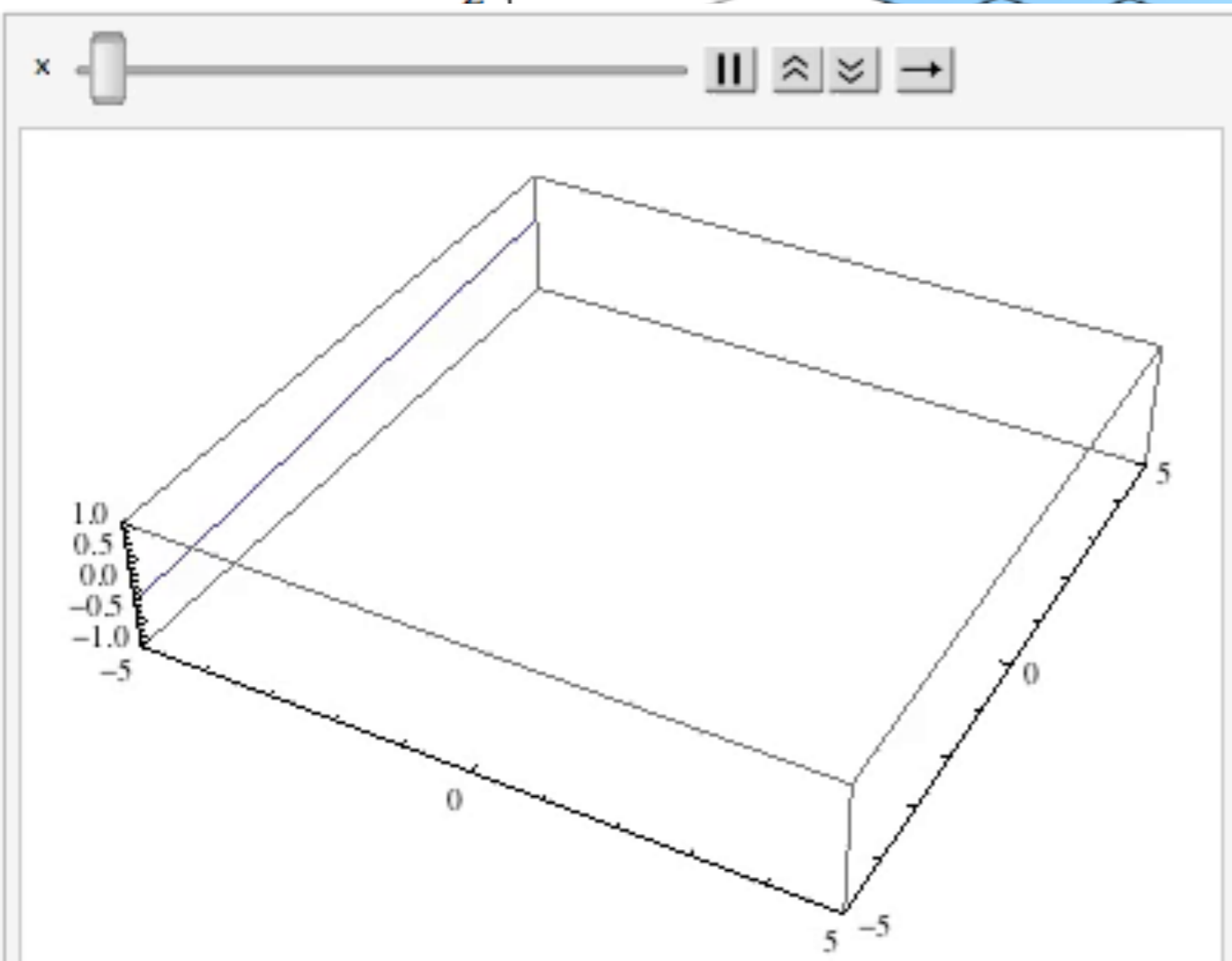
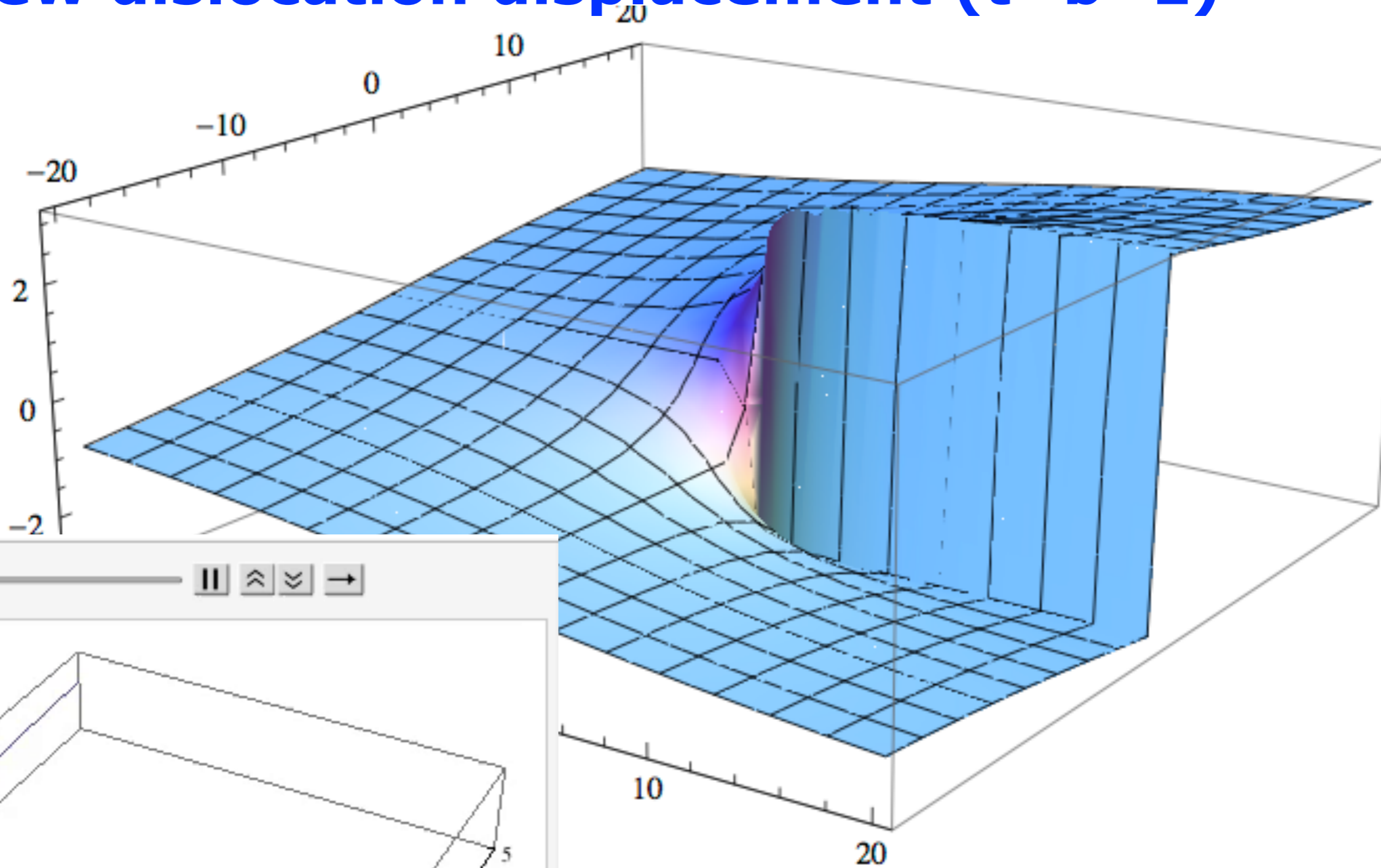
Edge / screw dislocation intersection

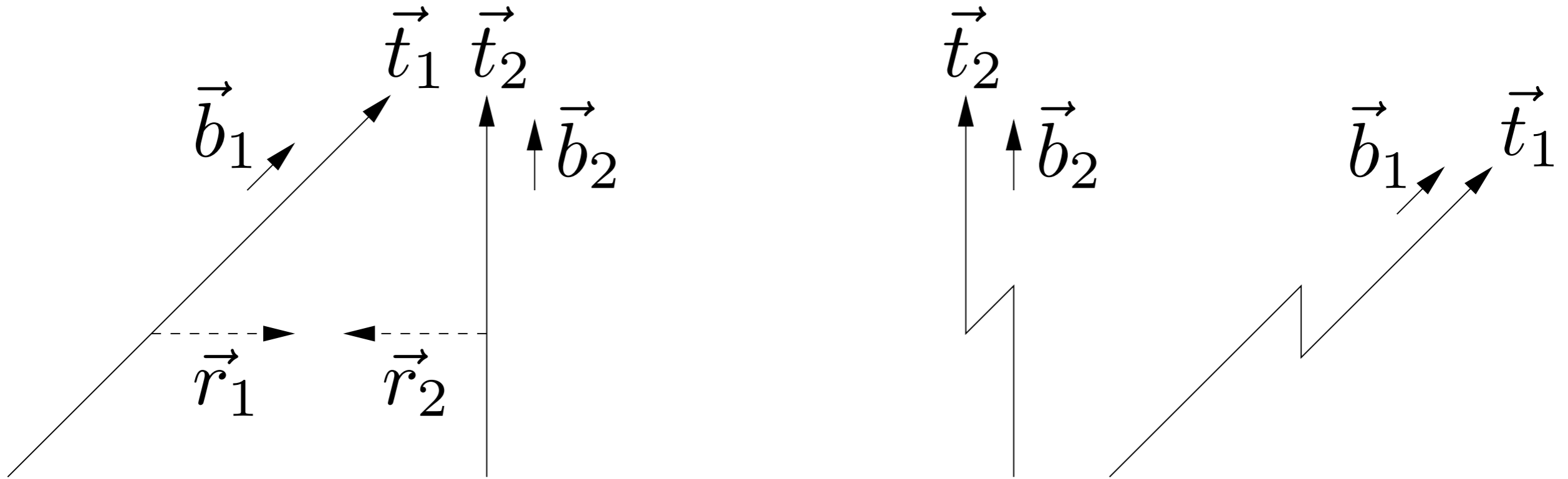


Screw / screw dislocation intersection



Screw dislocation displacement ($t=b=z$)





$$\vec{j}_1 = \vec{b}_2 \left[\frac{\vec{t}_1 \cdot (\vec{r}_1 \times \vec{t}_2)}{|\vec{t}_1 \cdot (\vec{r}_1 \times \vec{t}_2)|} \right]$$

$$\vec{j}_2 = \vec{b}_1 \left[\frac{\vec{t}_2 \cdot (\vec{r}_2 \times \vec{t}_1)}{|\vec{t}_2 \cdot (\vec{r}_2 \times \vec{t}_1)|} \right]$$

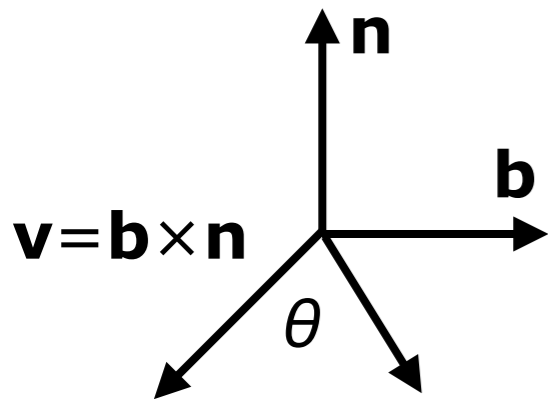
Dislocations in crystals to plasticity

- Dislocations in particular crystal structures: FCC, BCC, HCP, intermetallics
- Kinks and dislocation mobility
- Dislocation intersections and jogs

- Relationship between dislocation motion and plasticity

Dislocation motion under stress

- Force per length (“Peach-Kohler force”)
 - Always perpendicular to dislocation line
 - Force **in slip plane**: *glide force*
 - Force **normal to slip plane**: *climb force* (edge) or *cross-slip* (screw)



$$\mathbf{t} = \mathbf{v} \cos \theta + \mathbf{b} \sin \theta$$

glide force

cross-slip force

climb force

$$d\mathbf{F} = (\underline{\sigma} \cdot \mathbf{b}) \times d\mathbf{t}$$

$$= \begin{pmatrix} \sigma_{vv} & \sigma_{vb} & \sigma_{vn} \\ \sigma_{vb} & \sigma_{bb} & \sigma_{bn} \\ \sigma_{vn} & \sigma_{bn} & \sigma_{nn} \end{pmatrix} \cdot \begin{pmatrix} 0 \\ b \\ 0 \end{pmatrix} \times \begin{pmatrix} \cos \theta \\ \sin \theta \\ 0 \end{pmatrix} dt$$

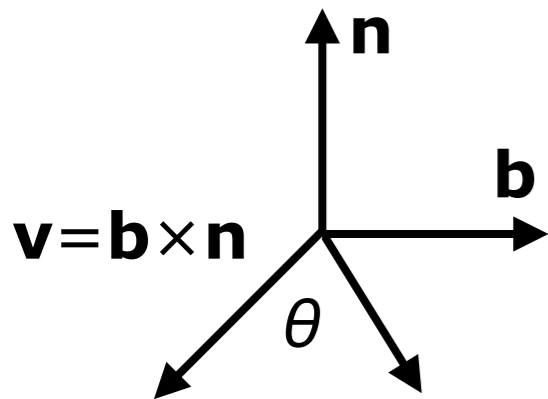
$$= \begin{pmatrix} \sigma_{bv}b \\ \sigma_{bb}b \\ \sigma_{bn}b \end{pmatrix} \times \begin{pmatrix} \cos \theta \\ \sin \theta \\ 0 \end{pmatrix} dt$$

$$= \begin{vmatrix} \mathbf{v} & \mathbf{b} & \mathbf{n} \\ \sigma_{bv}b & \sigma_{bb}b & \sigma_{bn}b \\ \cos \theta & \sin \theta & 0 \end{vmatrix} dt$$

$$= \sigma_{bn}b(-\mathbf{v} \sin \theta + \mathbf{b} \cos \theta) + \sigma_{bv}b \sin \theta \mathbf{n} - \sigma_{bb}b \cos \theta \mathbf{n}$$

Force on an edge and screw dislocation

- Force per length (“Peach-Kohler force”)
 - Always perpendicular to dislocation line
 - Force **in slip plane**: *glide force*
 - Force **normal to slip plane**: *climb force* (edge) or *cross-slip* (screw)



$$\mathbf{t} = \mathbf{v} \cos \theta + \mathbf{b} \sin \theta$$

$$\mathbf{dF} = \sigma_{bn} b (-\mathbf{v} \sin \theta + \mathbf{b} \cos \theta) + \sigma_{bv} b \sin \theta \mathbf{n} - \sigma_{bb} b \cos \theta \mathbf{n}$$

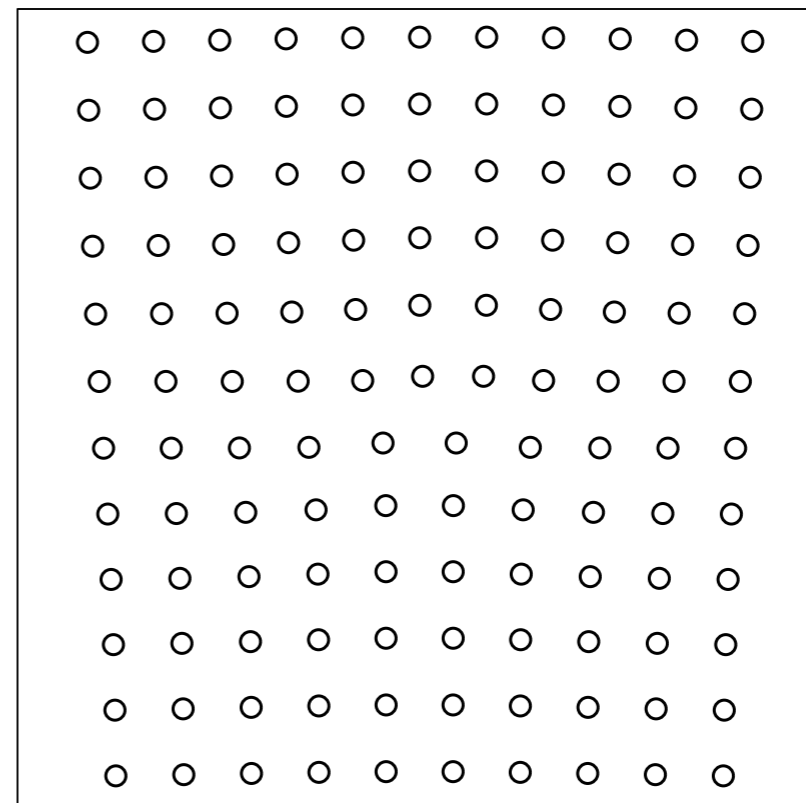
$$\mathbf{dF}_{\text{edge}} = \sigma_{bn} b \mathbf{b} - \sigma_{bb} b \mathbf{n}$$

$$\mathbf{dF}_{\text{screw}} = -\sigma_{bn} b \mathbf{v} + \sigma_{bv} b \mathbf{n}$$

glide force

cross-slip force

climb force



Crystal structure	Slip planes	Slip directions	Number of slip systems
Face-centered cubic	$\{111\} \times 4$	$\langle 1\bar{1}0 \rangle \times 3$	$4 \times 3 = 12$
Body-centered cubic	$\{110\} \times 6$	$\langle \bar{1}11 \rangle \times 2$	$6 \times 2 = 12$
	$\{211\} \times 12$	$\langle \bar{1}11 \rangle \times 1^*$	$12 \times 1 = 12$
	$\{321\} \times 24$	$\langle \bar{1}11 \rangle \times 1^*$	$24 \times 1 = 24$
Hexagonal-closed packed	$\{0001\} \times 1$	$\langle 11\bar{2}0 \rangle \times 3$	$1 \times 3 = 3$
	$\{10\bar{1}0\} \times 3$	$\langle 11\bar{2}0 \rangle \times 1$	$3 \times 1 = 3$
	$\{10\bar{1}1\} \times 6$	$\langle 11\bar{2}0 \rangle \times 1$	$6 \times 1 = 6$

*sign of slip direction important

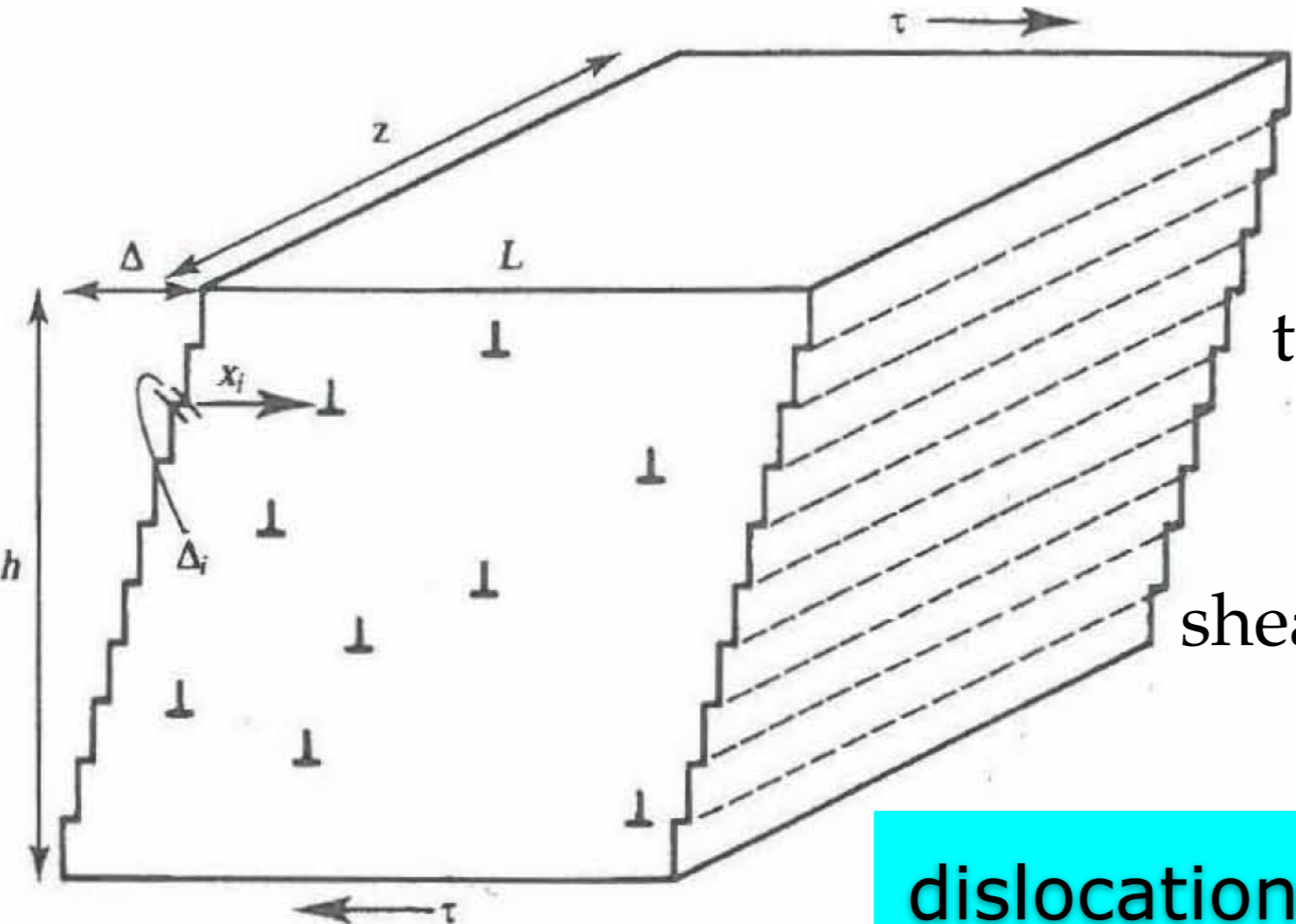
$$\underline{\varepsilon} = \gamma \begin{pmatrix} b_x n_x & \frac{1}{2}(b_x n_y + b_y n_x) & \frac{1}{2}(b_x n_z + b_z n_x) \\ \frac{1}{2}(b_x n_y + b_y n_x) & b_y n_y & \frac{1}{2}(b_y n_z + b_z n_y) \\ \frac{1}{2}(b_x n_z + b_z n_x) & \frac{1}{2}(b_y n_z + b_z n_y) & b_z n_z \end{pmatrix}$$

FCC: Al, Cu, Ni, Ag, Au ...

BCC: Fe, Nb, Mo, Ta, W ...

HCP: Zn, Cd, Mg, Ti, Zr ...

Dislocation motion



slip: $\Delta_i = b \frac{x_i}{L}$

total slip: $\Delta = \sum_{i=1}^{N_{\perp}} \Delta_i = \frac{b}{L} \sum_{i=1}^{N_{\perp}} x_i$

shear strain: $\gamma \approx \frac{\Delta}{h} = \frac{b}{hL} \sum_{i=1}^{N_{\perp}} x_i$

dislocation density

average dislocation displacement

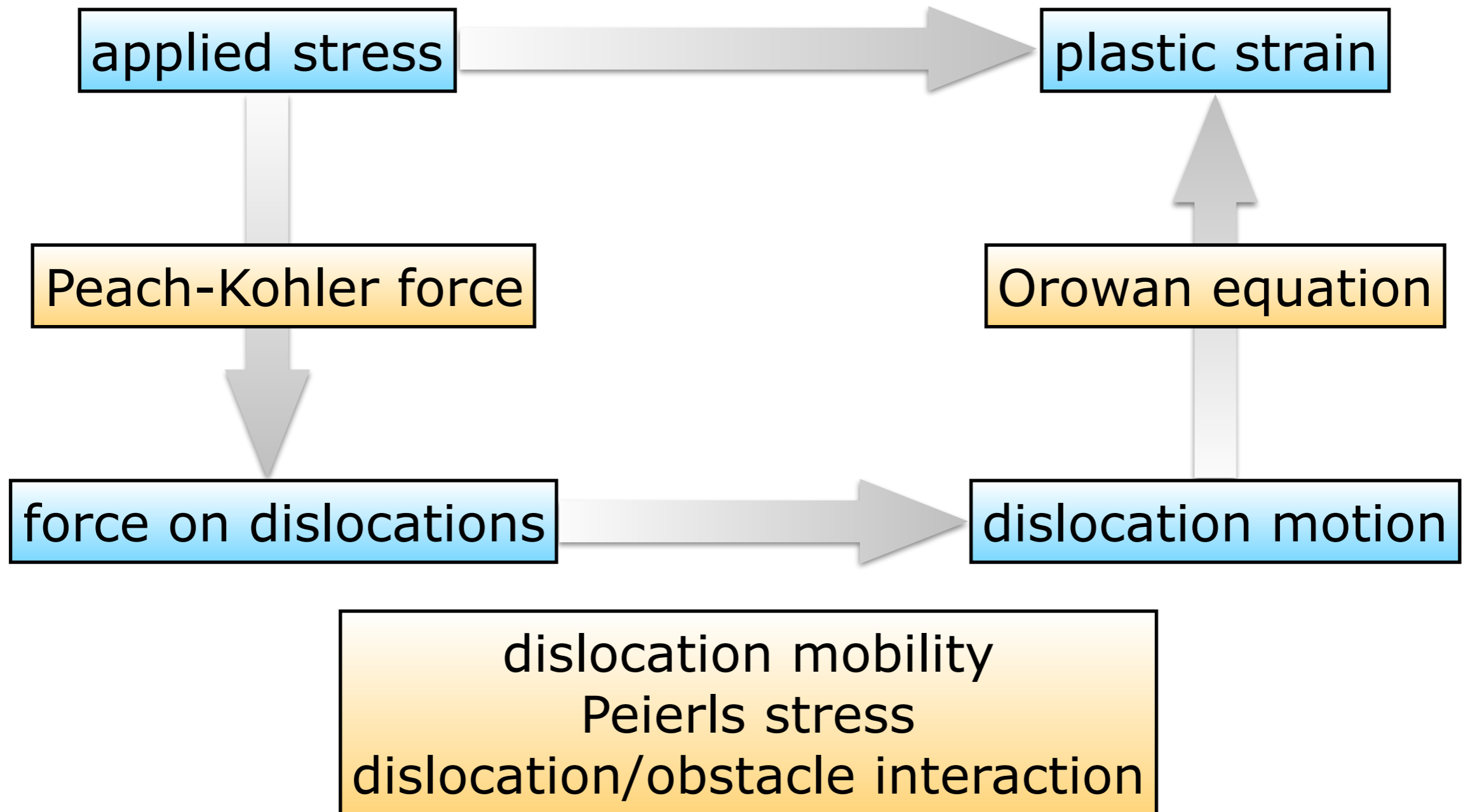
$$= \frac{bN_{\perp}}{hL} \frac{1}{N_{\perp}} \sum_{i=1}^{N_{\perp}} x_i$$

Two competing effects as plastic strain increases:
 ρ_{\perp} increases \rightarrow suggests *softening* (e.g., yield point)
 v_{\perp} decreases \rightarrow suggests *hardening* (e.g., all others)

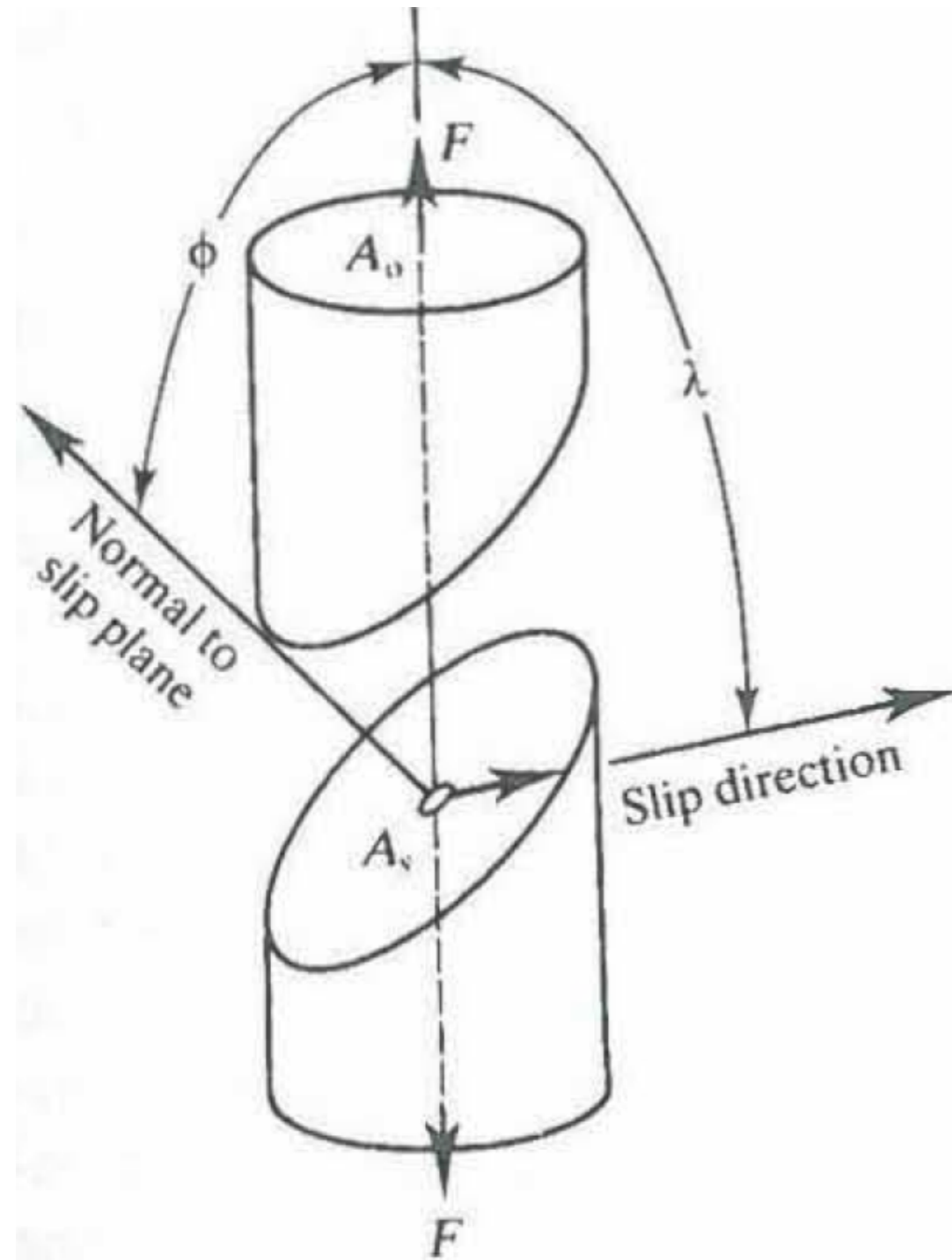
$$\gamma = b\rho_{\perp}\bar{x}_{\perp}$$

$$\dot{\gamma} = b\rho_{\perp}\bar{v}_{\perp}$$

Dislocations and plastic deformation



- Resolved shear stress: computing σ_{bn} for a particular slip system.



$$\tau_{RSS} = \frac{\text{(force resolved in slip direction)}}{\text{(area of slip plane)}}$$

$$= \frac{F \cos \lambda}{A / \cos \phi} = \frac{F}{A} \cos \phi \cos \lambda$$

$$\frac{1}{m} = \cos \phi \cos \lambda = M \leq \frac{1}{2}$$

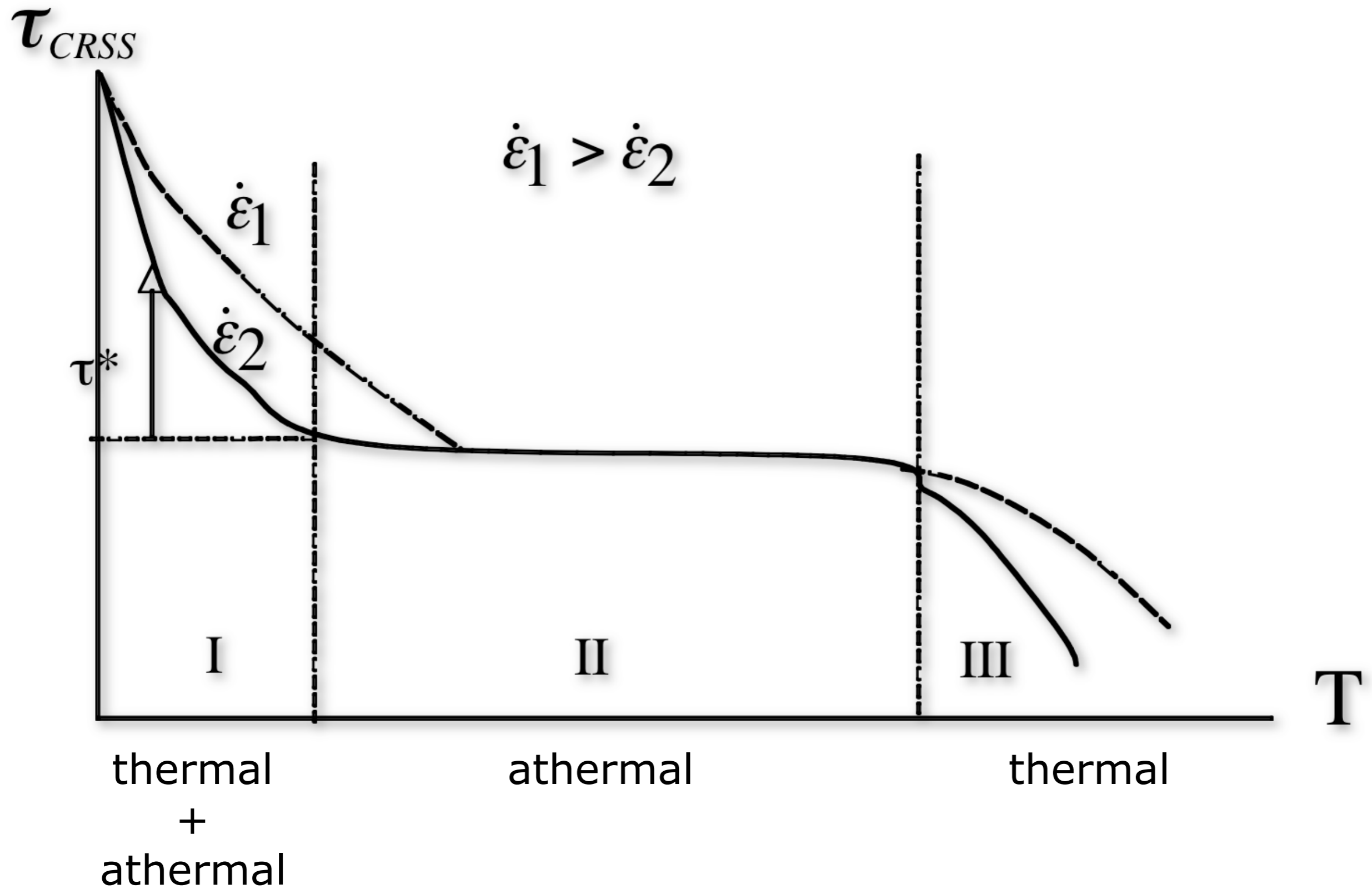
$$\cos \phi = \hat{\mathbf{F}} \cdot \hat{\mathbf{n}} = \frac{\mathbf{F} \cdot \mathbf{n}}{|\mathbf{F}| |\mathbf{n}|}$$

$$\cos \lambda = \hat{\mathbf{F}} \cdot \hat{\mathbf{b}} = \frac{\mathbf{F} \cdot \mathbf{b}}{|\mathbf{F}| |\mathbf{b}|}$$

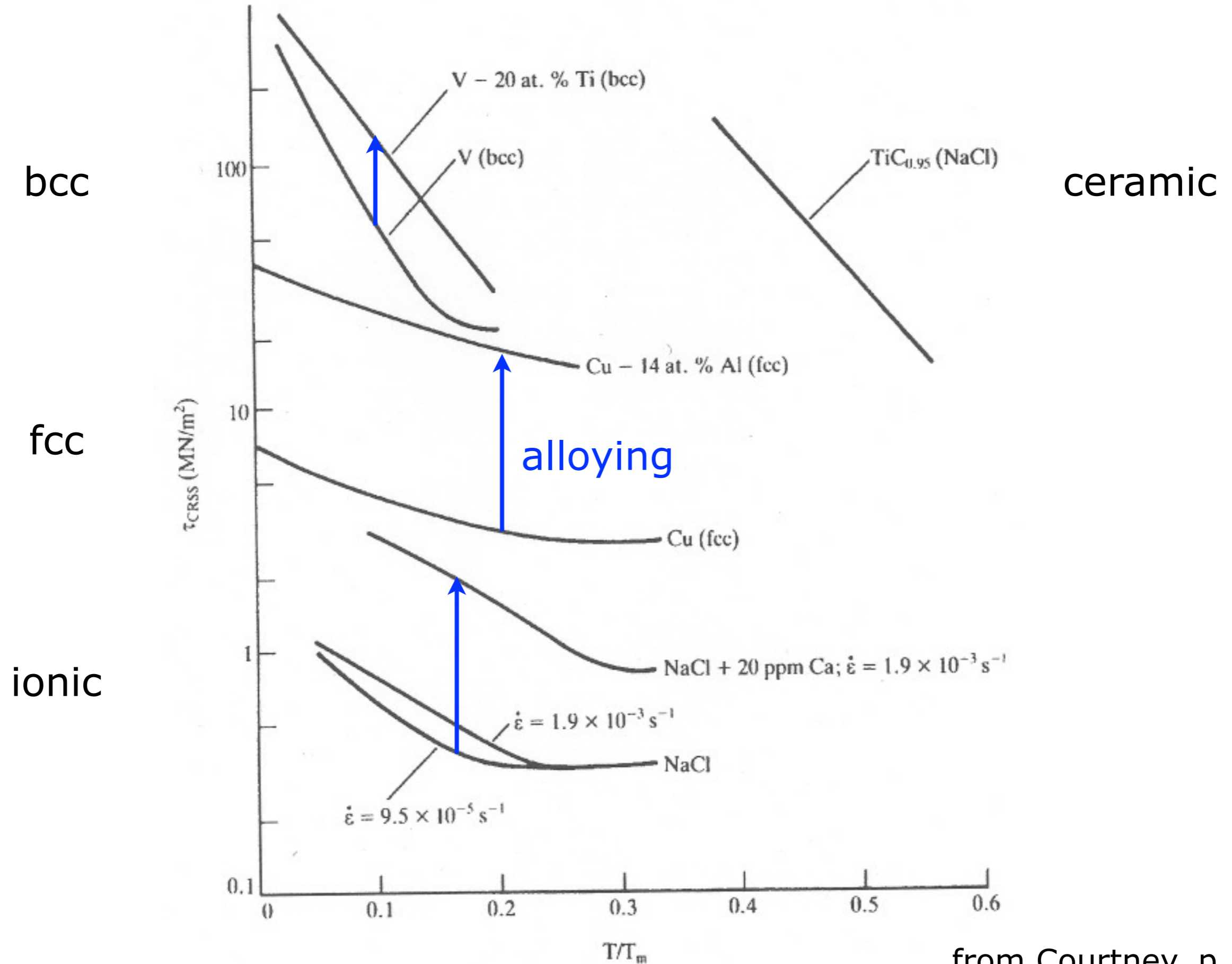
$$M = (\hat{\mathbf{F}} \cdot \hat{\mathbf{n}})(\hat{\mathbf{F}} \cdot \hat{\mathbf{b}}) = \frac{(\mathbf{F} \cdot \mathbf{n})(\mathbf{F} \cdot \mathbf{b})}{|\mathbf{F}|^2 |\mathbf{n}| |\mathbf{b}|}$$

$$\sigma_{YS} = m \tau_{CRSS}$$

CRSS with temperature and strain rate



CRSS with temperature and material



Plasticity to solute strengthening

- Relationship between dislocation motion and plasticity
- Solute-dislocation interactions
- Solid solution strengthening

Solutes and dislocations: How they do?

Solutes interact by **changing matrix properties**

- different atomic size (**elastic** interaction)
- different bond stiffness (**modulus** interaction)
- different stacking fault energy (**chemical** interaction)
- different charge (**electrostatic** interaction)
- different short-range ordering preference
- messing up long-range order (intermetallics)

All result in change in dislocation energy that is solute/dislocation position dependent.

$$\vec{F} = -\nabla E$$

Strengthening via solid solutions

- Impurity atoms distort the lattice & generate stress.
- Stress can produce a barrier to dislocation motion.

Smaller impurity atoms

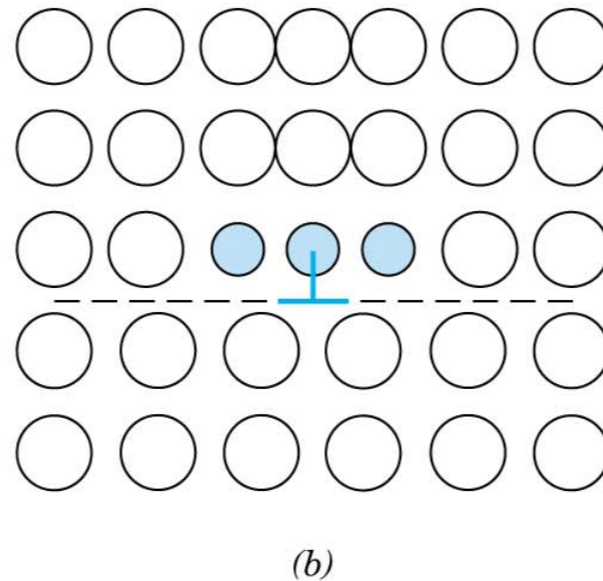
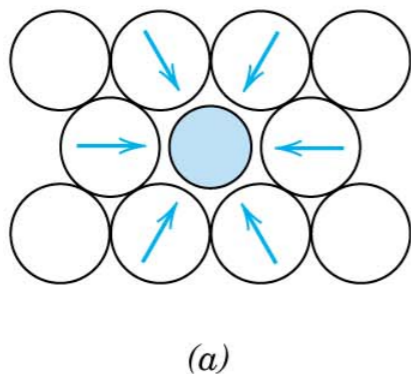


FIGURE 7.15

(a) Representation of tensile lattice strains imposed on host atoms by a smaller substitutional impurity atom. (b) Possible locations of smaller impurity atoms relative to an edge dislocation such that there is partial cancellation of impurity–dislocation lattice strains.

Larger impurity atoms

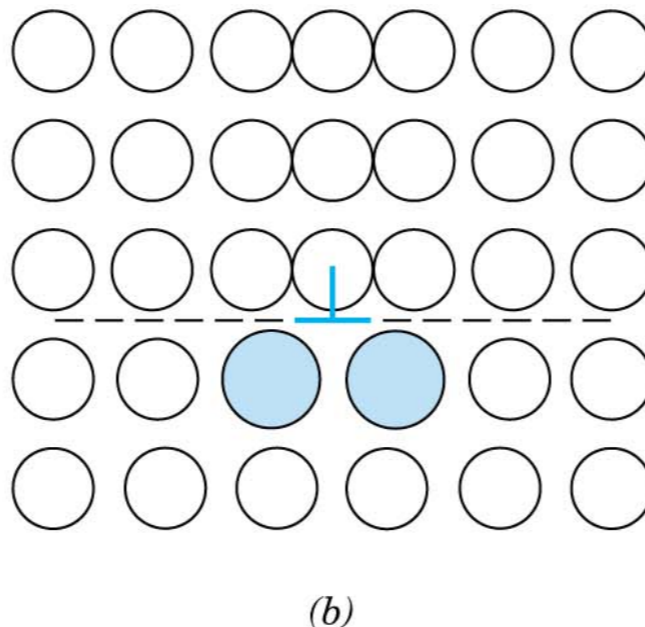
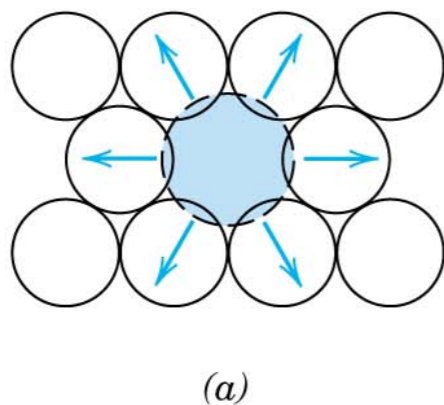


FIGURE 7.16

(a) Representation of compressive strains imposed on host atoms by a larger substitutional impurity atom. (b) Possible locations of larger impurity atoms relative to an edge dislocation such that there is partial cancellation of impurity–dislocation lattice strains.

Edge dislocation: Stress field

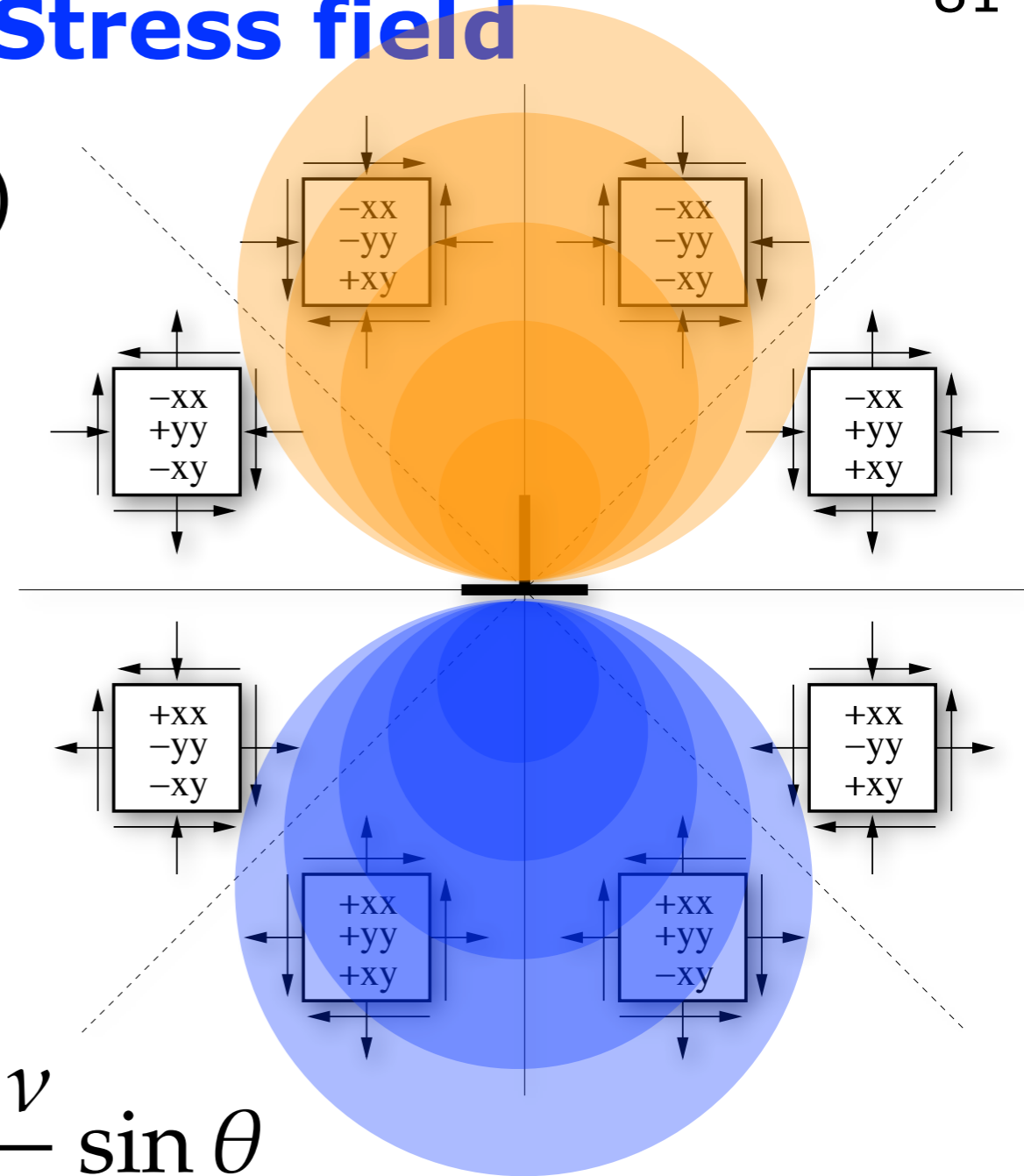
$$\sigma_{xx} = -\frac{Gb}{2\pi r(1-\nu)} \sin \theta (2 + \cos 2\theta)$$

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

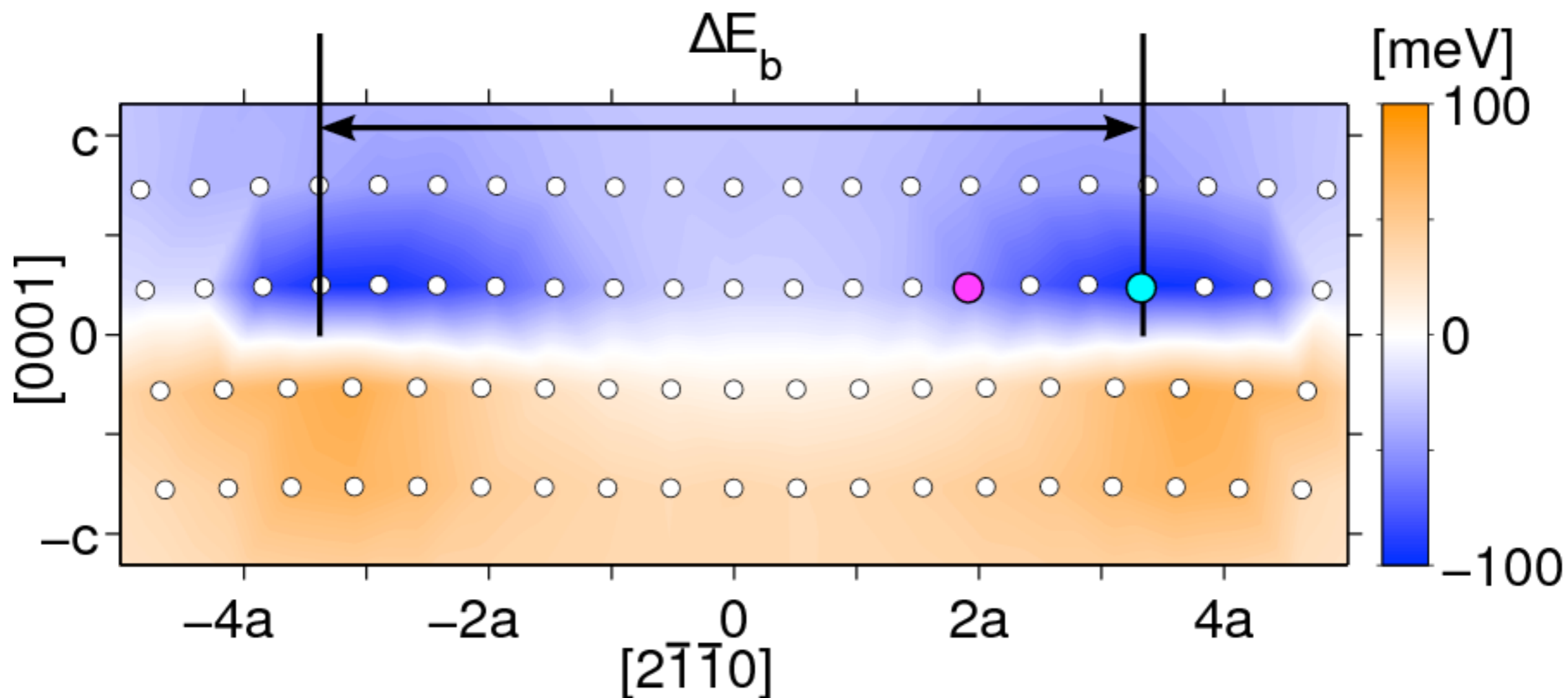
$$\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$$

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

$$\begin{aligned} p &= \frac{1}{3} (\sigma_{xx} + \sigma_{yy} + \sigma_{zz}) = -\frac{Gb}{3\pi r} \frac{1+\nu}{1-\nu} \sin \theta \\ &= -K \frac{b}{2\pi r} \frac{1-2\nu}{1-\nu} \sin \theta \\ &\approx -K \frac{b}{4\pi r} \sin \theta \end{aligned}$$

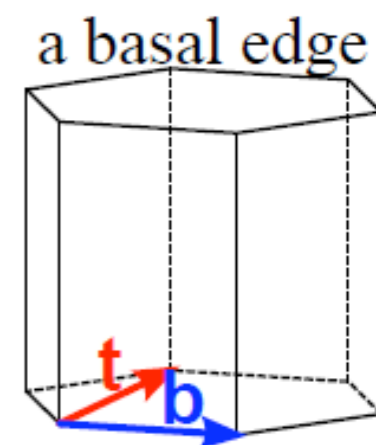


Aluminum in magnesium edge dislocation

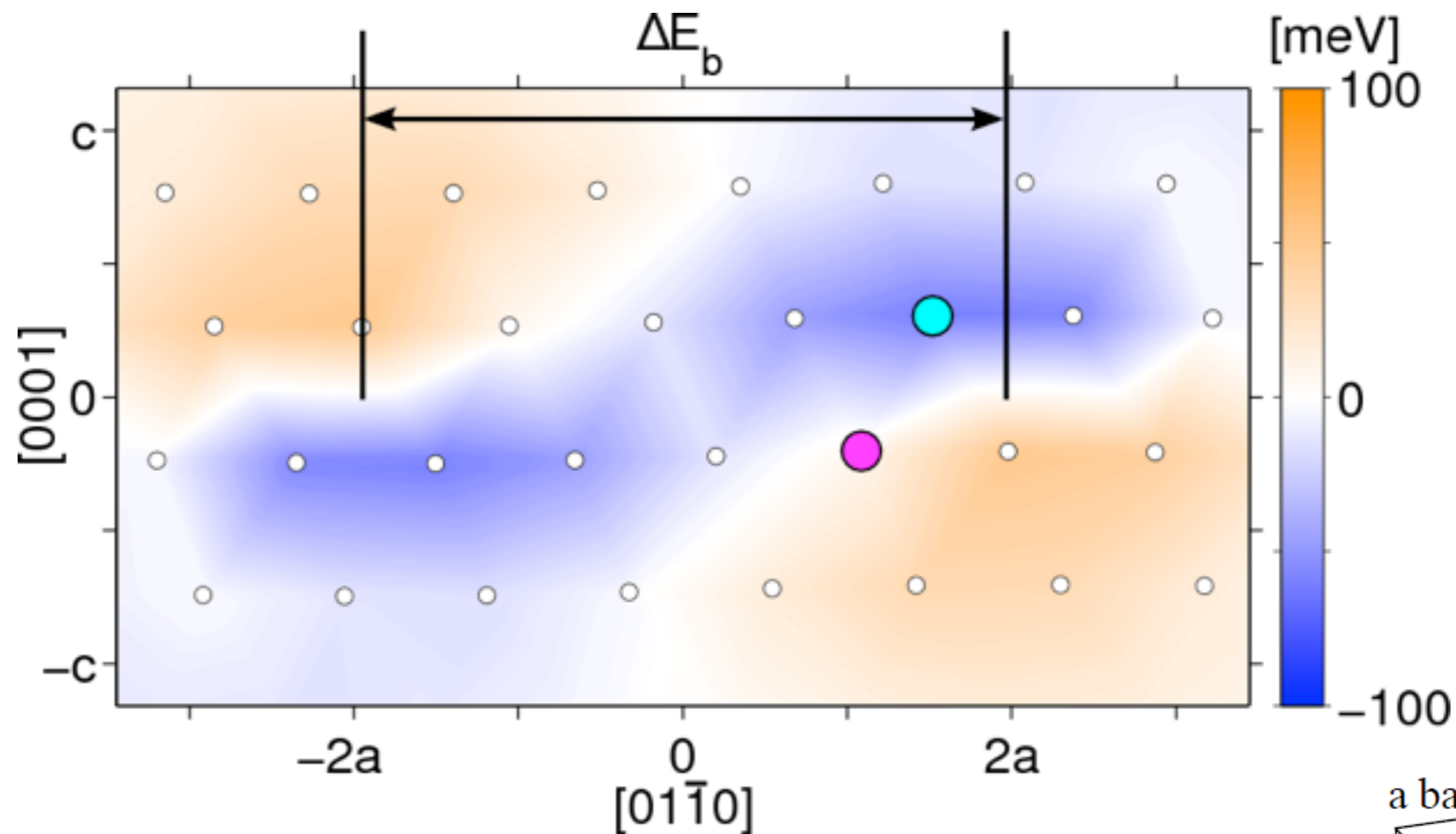


● maximum $\Delta E_b = 99.2$ meV.

● $F_{\max} = \partial_x \Delta E_b = 12.3$ meV/Å resistive force to glide past solute



Aluminum in magnesium screw dislocation

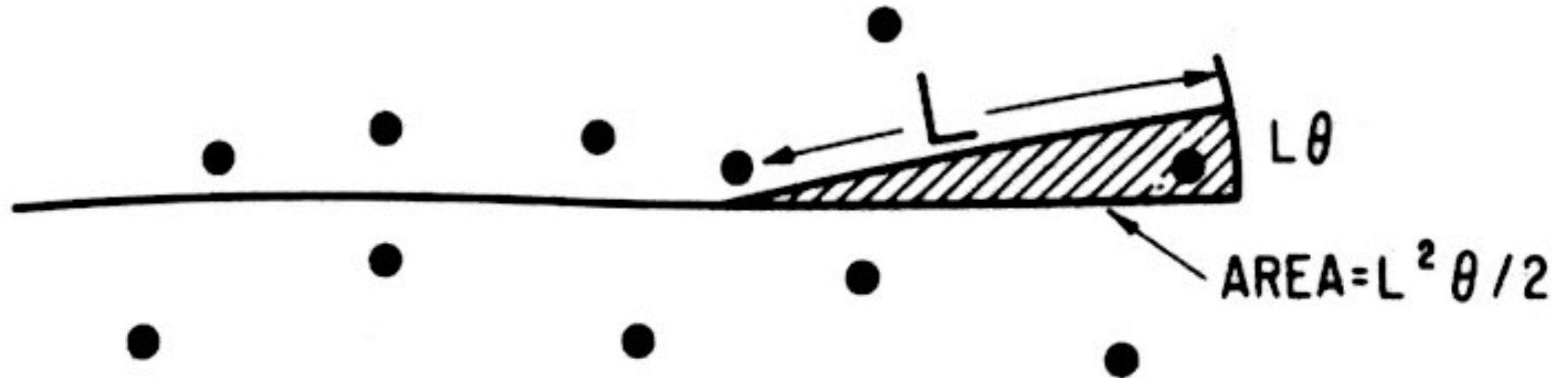


● maximum $\Delta E_b = 59.6$ meV.

● $F_{\max} = \partial_x \Delta E_b = 11.4$ meV/Å resistive force to glide past solute

Solute strengthening from **both** edge and screw dislocations

Dilute solute strengthening: Weak obstacles



- Peach-Koehler force (τb) balances solute resistance (F_{\max}) when the dislocation becomes unpinned: $\tau b = F_{\max}/L$

- Line tension (E) balances F_{\max} as it becomes unpinned:

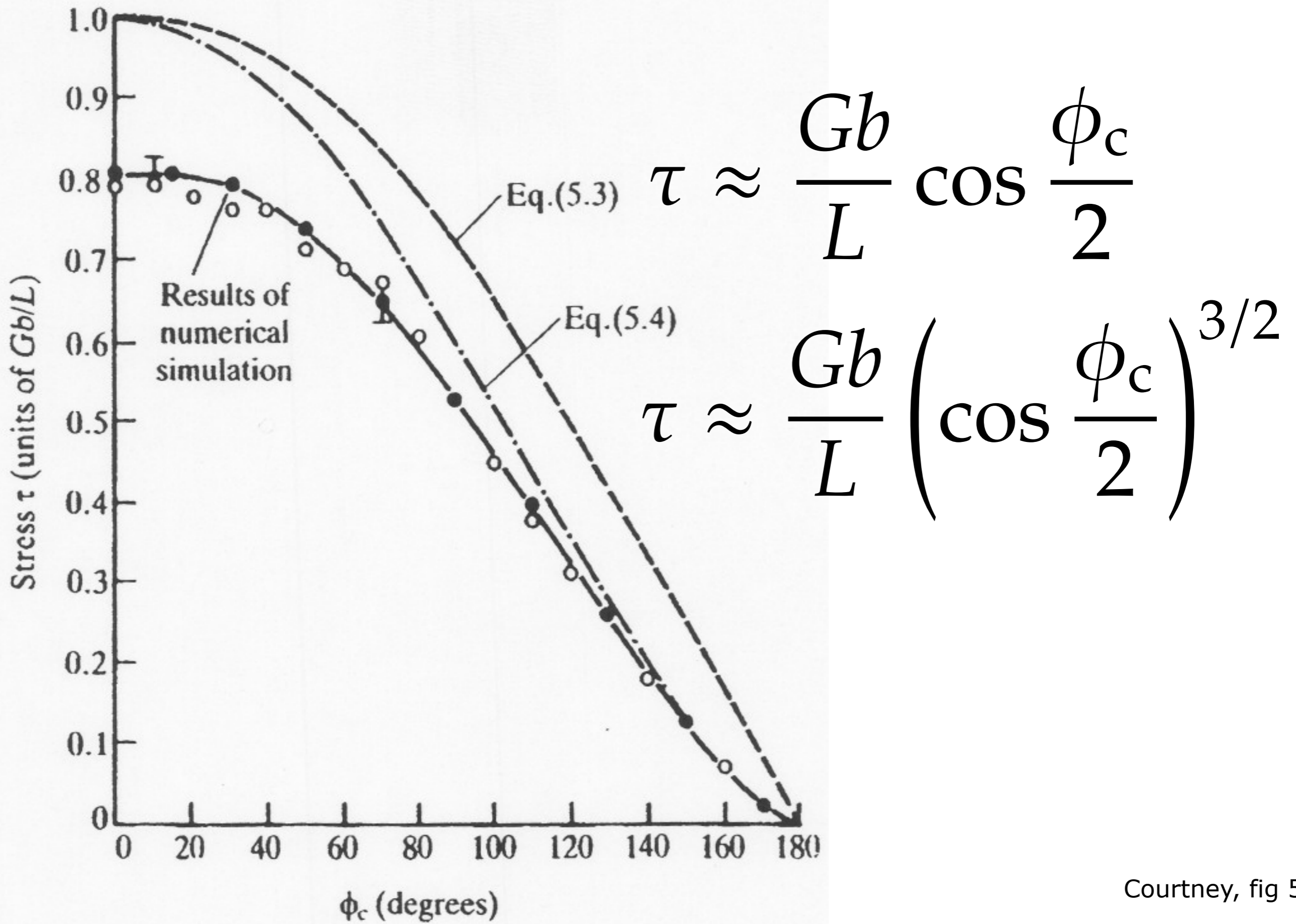
$$F_{\max} = 2E \sin(\theta) \approx 2E\theta$$

- Mean spacing of random solutes: $L = \frac{\sqrt[4]{3}}{4} \sqrt{\frac{\pi}{c\theta}} b$ c: solute conc.
b: Burgers vector

$$\Delta\tau = \frac{2}{(3\pi^2)^{1/4}} \frac{E}{b^2} \left(\frac{F_{\max}}{E} \right)^{3/2} c^{1/2}$$

- Solute strengthening scales as $(F_{\max})^{3/2}$ and $c^{1/2}$
- F_{\max} can be determined computationally, or with simple models.

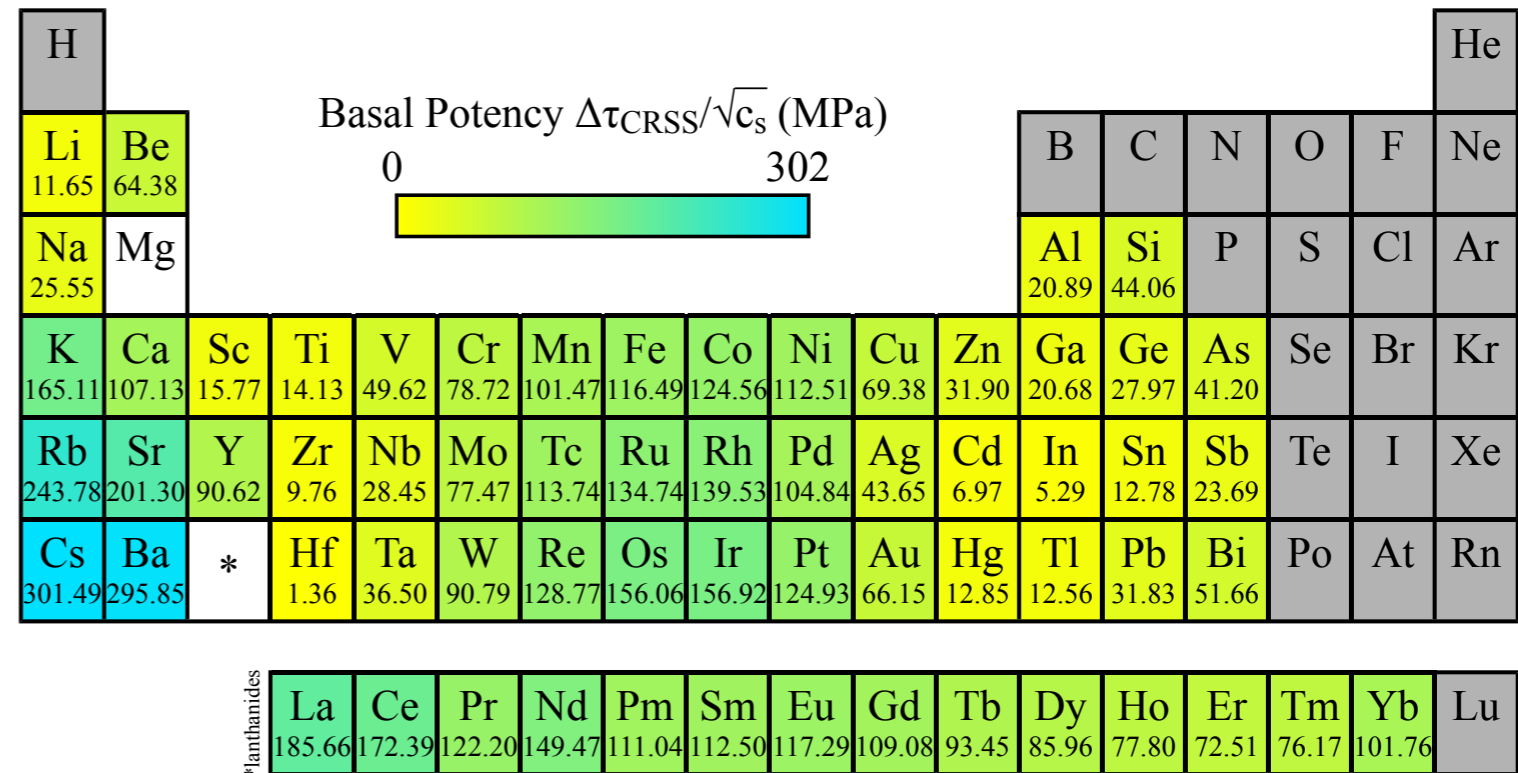
Strength vs. critical bowing angle



Basal strengthening for Mg from first-principles⁸⁶

$$\Delta\tau_{\text{CRSS}(0001)} = \left[0.30 (F_{\text{max}}^{\text{screw}})^{3/2} + 0.22 (F_{\text{max}}^{\text{edge}})^{3/2} \right] \cdot c^{1/2}$$

Solute	Exp $\Delta\tau/c^{1/2}$	Model $\Delta\tau/c^{1/2}$
Al	21.2 MPa	19.6 MPa
Zn	31.1	32.7
In	9.02	7.5
Cd	6.03	5.3
Li	11.2	14.4
Tl	8.25	10.8
Pb	>14.0	40.1
Sn	24.3	17.1
Bi	>25.0	60.6



Completely first-principles **design map** for solute strengthening

1. Akhtar and Teghtsoonian (1969)
3. Scharf et al. (1968)
5. Levine et al. (1959)

2. Akhtar and Teghtsoonian (1971)
4. Yoshinaga and Horiuchi (1963)
6. Van der Planken and Deruyttere (1969)

Yasi, Hector, Trinkle,
Acta Mater. **58**, 5704 (2010).

What if I don't have a fancy supercomputer? 87

- Simple “classical” (empirical) models have been around for decades
 - Interaction with stress field approximated by “size” and “modulus” misfit
 - **Size misfit:** difference in atomic radii (or change in lattice constant)
 - **Modulus misfit:** difference in “stiffness” (change in elastic constant)

spherical distortion: $\Delta\tau_{\text{CRSS}} \approx \frac{G\varepsilon_{\text{solute}}^{3/2}}{700} c^{1/2}$ $\varepsilon_{\text{solute}} = |\varepsilon'_G - \beta\varepsilon_b|$

$$\varepsilon'_G = \frac{\varepsilon_G}{1 + \frac{1}{2}|\varepsilon_G|}$$

$$\varepsilon_G = \frac{1}{G} \left. \frac{dG}{dc} \right|_{c=0}$$

$$\varepsilon_b = \frac{1}{b} \left. \frac{db}{dc} \right|_{c=0}$$

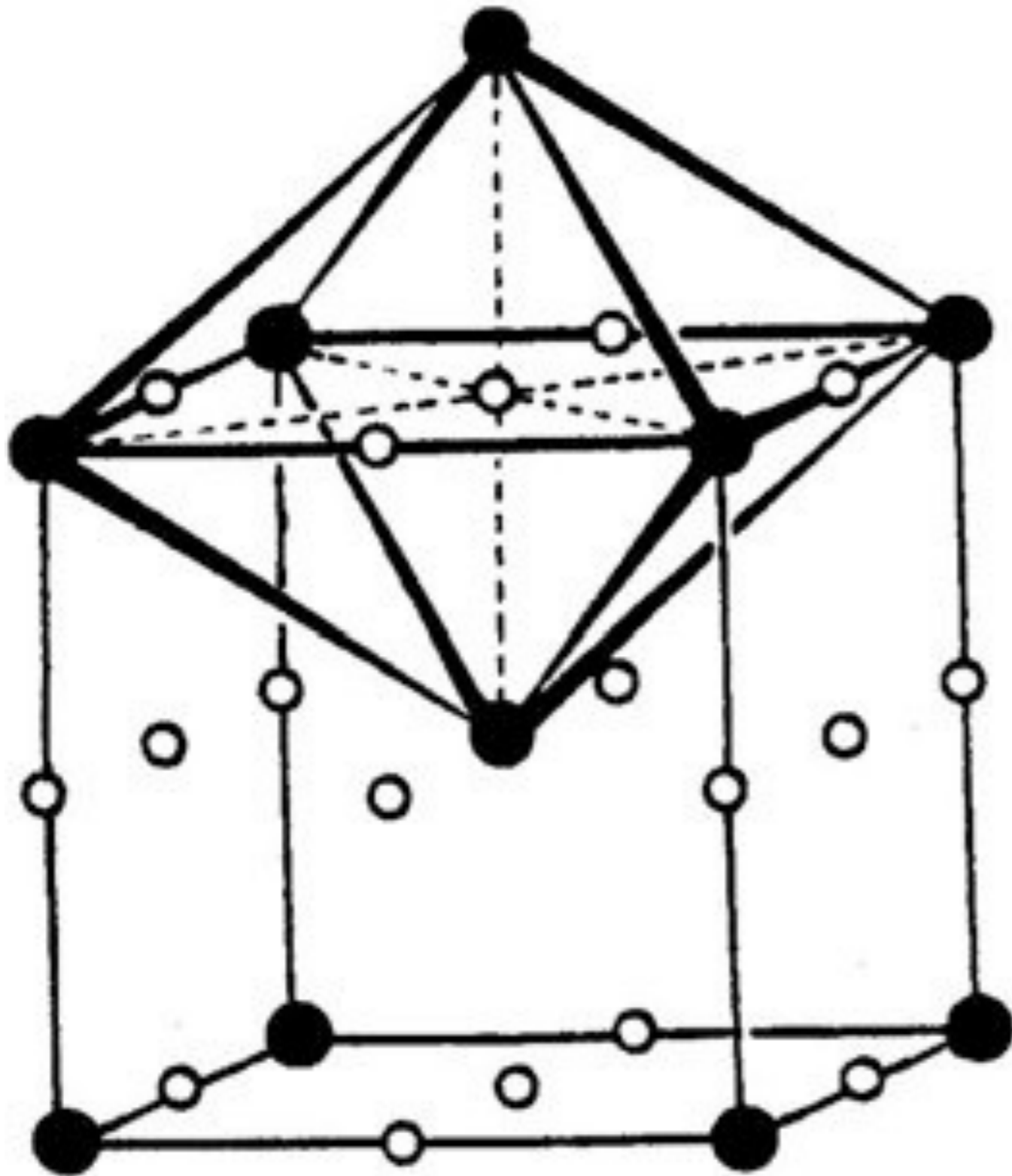
tetragonal distortion: $\Delta\tau_{\text{CRSS}} \approx \gamma Gc^{1/2}$ $\gamma \sim 1$

Octahedral interstitial sites in BCC

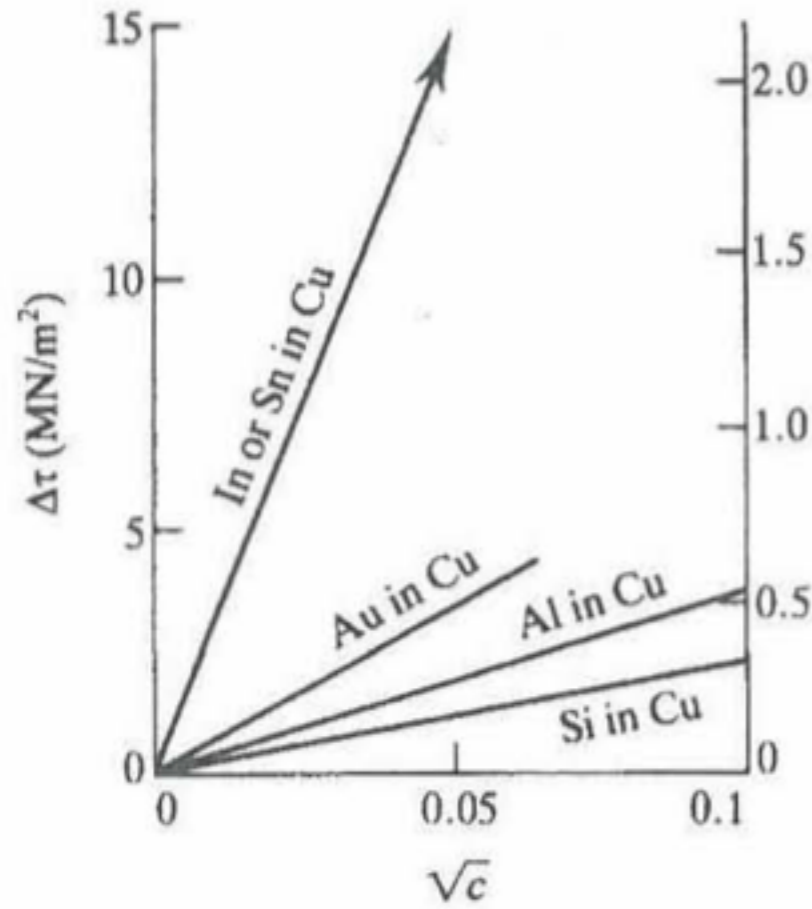
Interstitials (C, N, O) occupy octahedral sites on a BCC lattice

All sites are equivalent in an **unstrained** lattice

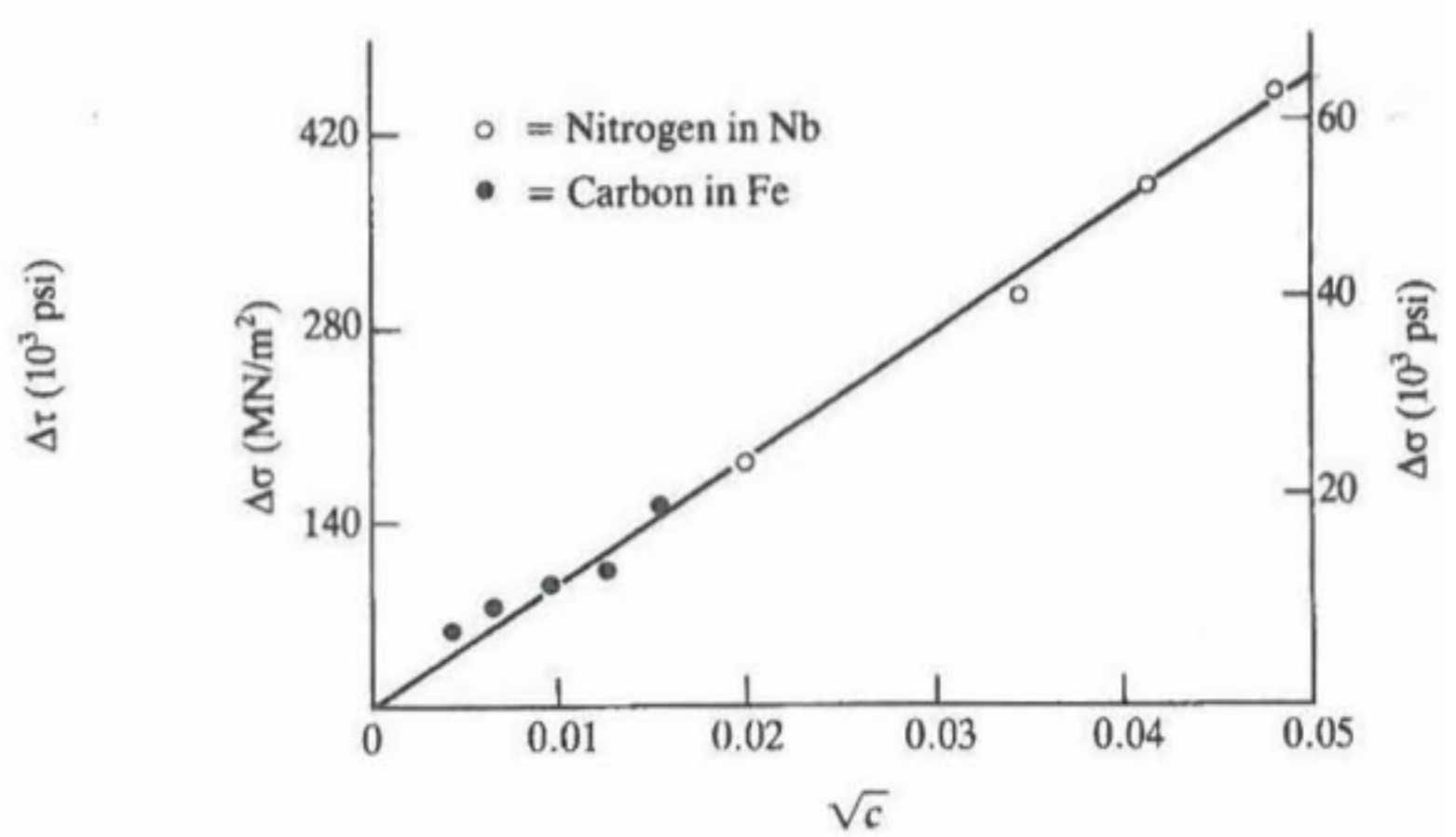
Strain along a $[100]$ axis breaks symmetry and can drive interstitial diffusion



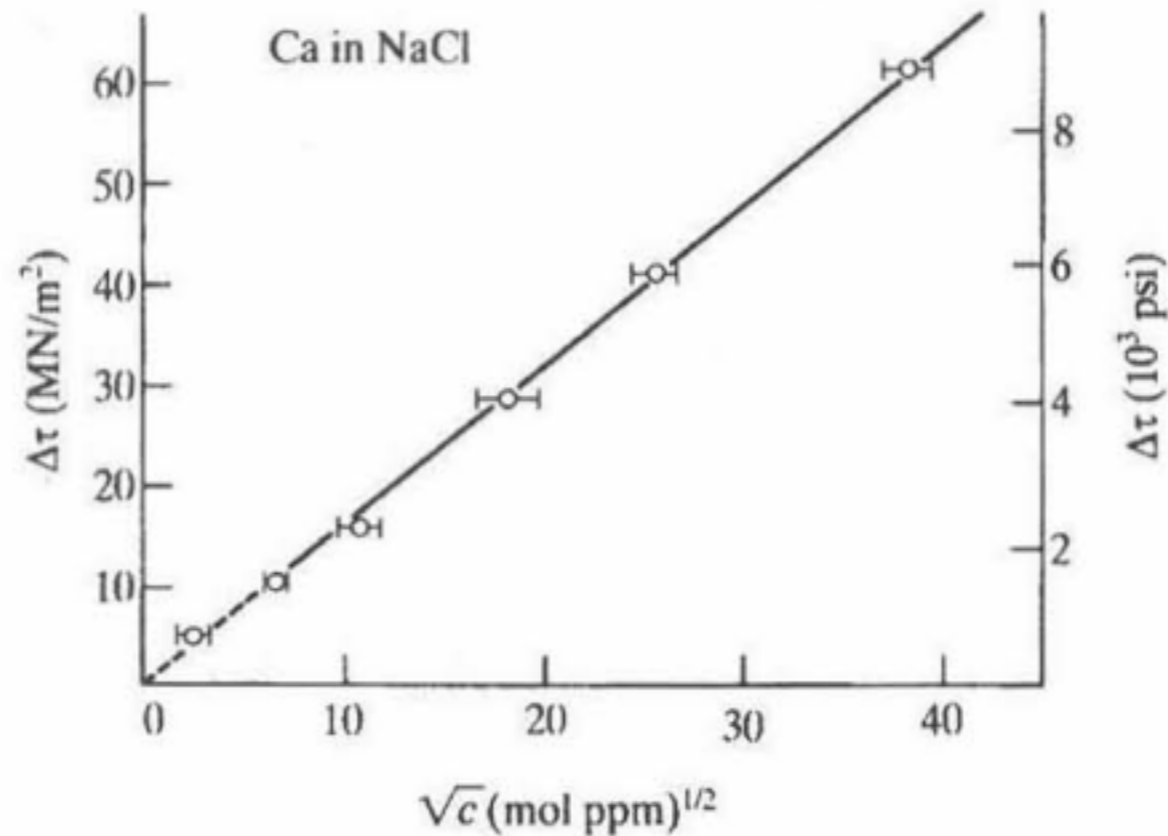
What if I don't have a fancy supercomputer? 89



(a)



(b)



Edge dislocation: Stress field

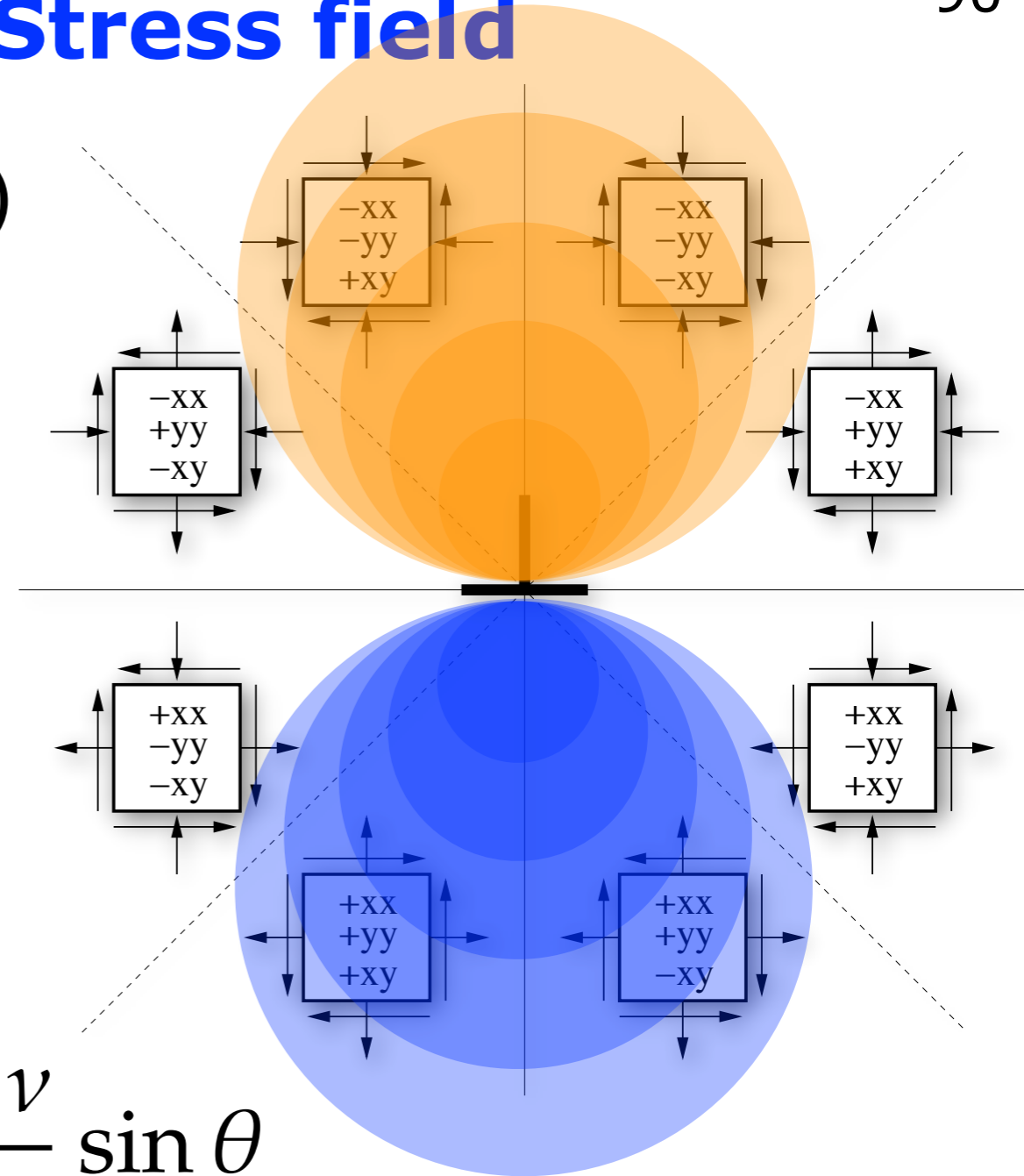
$$\sigma_{xx} = -\frac{Gb}{2\pi r(1-\nu)} \sin \theta (2 + \cos 2\theta)$$

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

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

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

$$\begin{aligned} p &= \frac{1}{3} (\sigma_{xx} + \sigma_{yy} + \sigma_{zz}) = -\frac{Gb}{3\pi r} \frac{1+\nu}{1-\nu} \sin \theta \\ &= -K \frac{b}{2\pi r} \frac{1-2\nu}{1-\nu} \sin \theta \\ &\approx -K \frac{b}{4\pi r} \sin \theta \end{aligned}$$



Solute strengthening to work-hardening

- Solute-dislocation interactions
- Solid solution strengthening

- Dislocations as obstacles
- Work-hardening stages

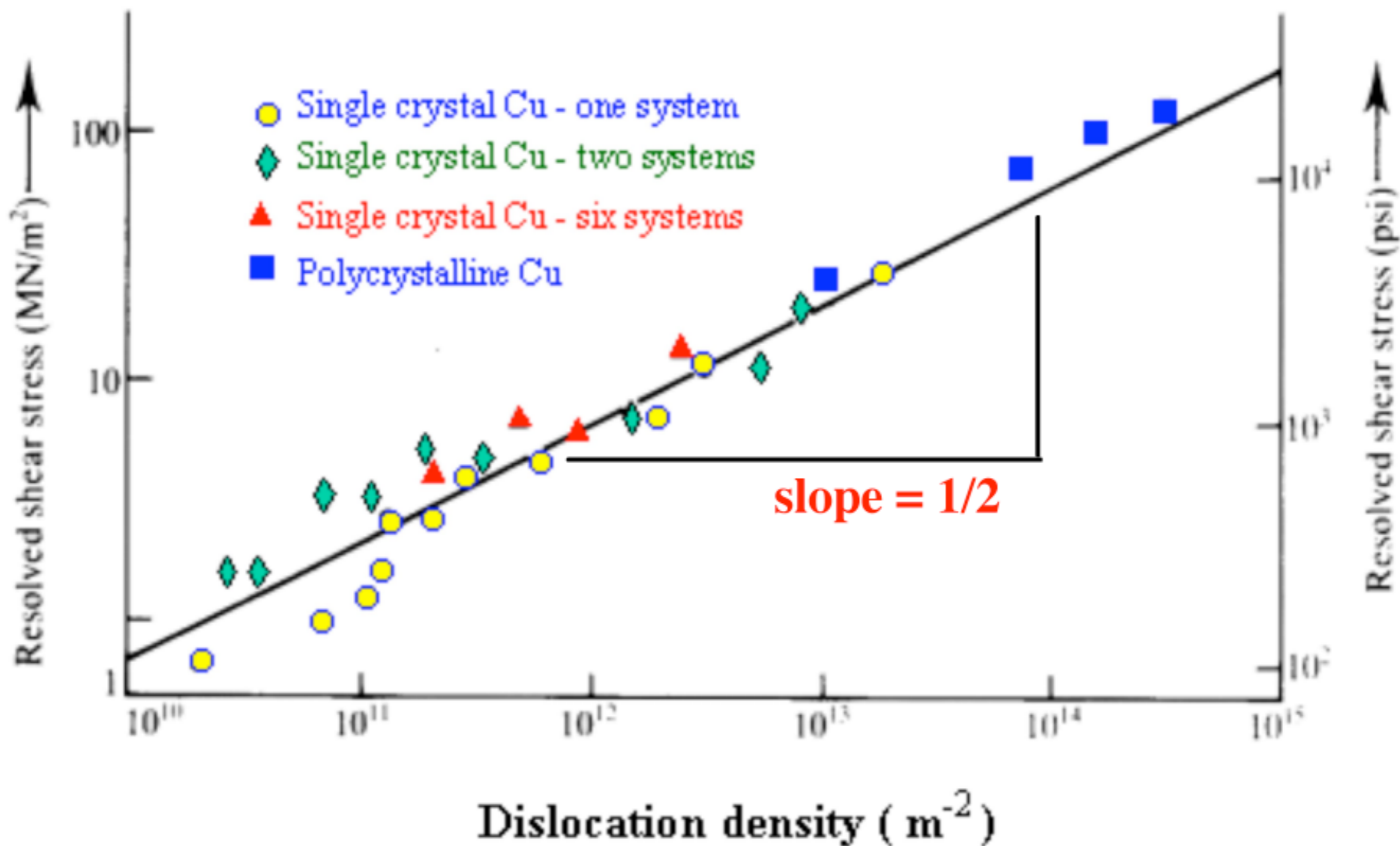
- Dislocations as obstacles
 - Stress fields of dislocations (low density)
 - Jogs created by intersections with “forest” dislocations (high density)
- Separation distance $L \approx \rho_{\perp}^{-1/2}$

$$\tau_{\text{CRSS}}^{\text{work-hardening}} = \tau_0 + \alpha Gb \sqrt{\rho_{\perp}} \quad \text{work-hardening rate: } \theta = \frac{d\tau}{d\gamma}$$

$$\alpha \approx \begin{cases} 0.2 & : \text{fcc} \\ 0.4 & : \text{bcc} \end{cases}$$

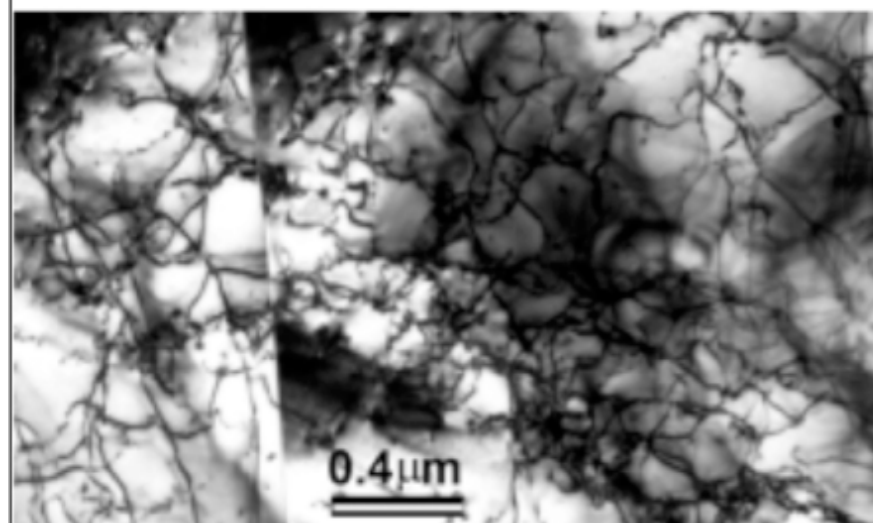
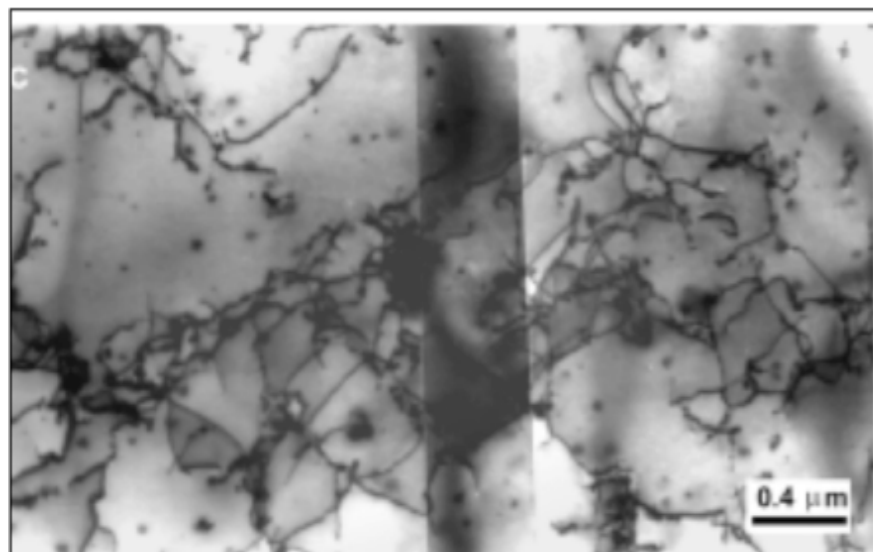
- Three stages of work-hardening:
 - Stage I: easy glide ($\theta \sim 10^{-4} G$)
 - single slip system, weak dislocation interactions
 - Stage II: linear hardening ($\theta \sim G/300$)
 - multiple slip, intersection from slip systems, jog formation
 - Stage III: exhaustion hardening (decreasing θ)
 - cross-slip to avoid obstacles, recovery mechanisms reduce ρ_{\perp}
 - formation of “cells” decreases elastic energy

Cu CRSS vs. dislocation density

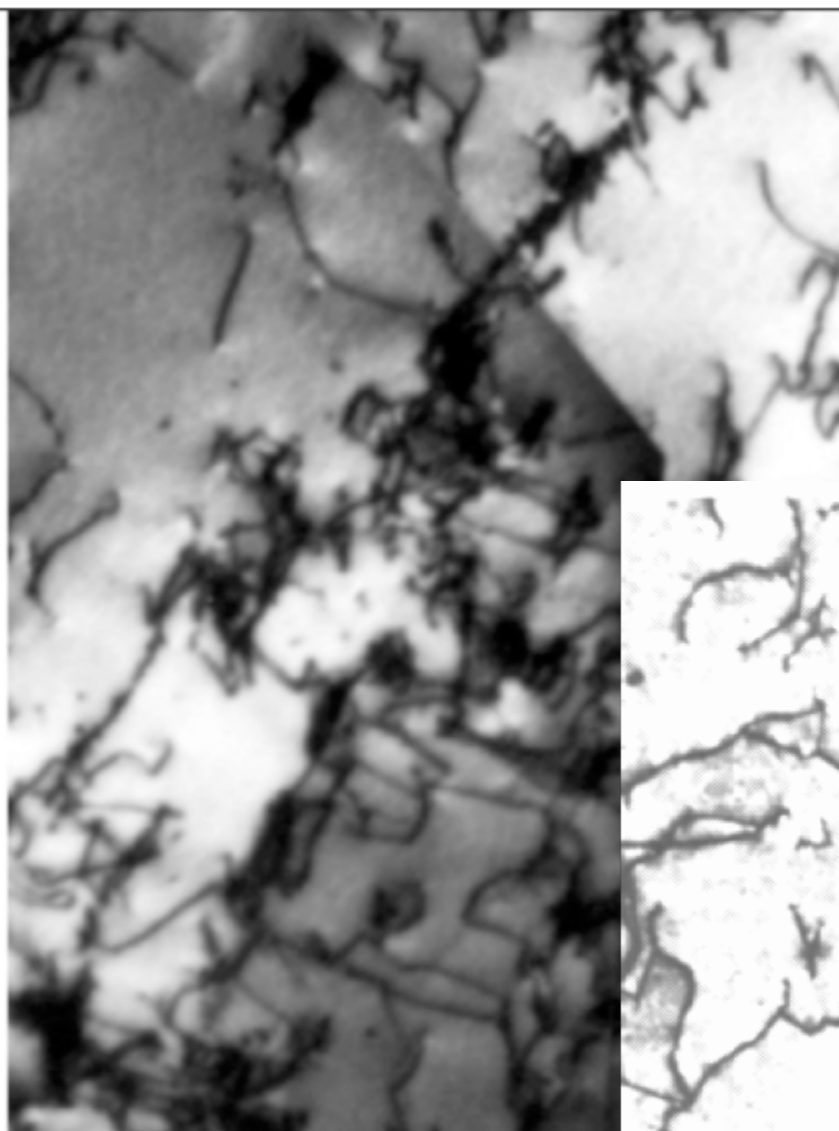


Cold-working microstructure

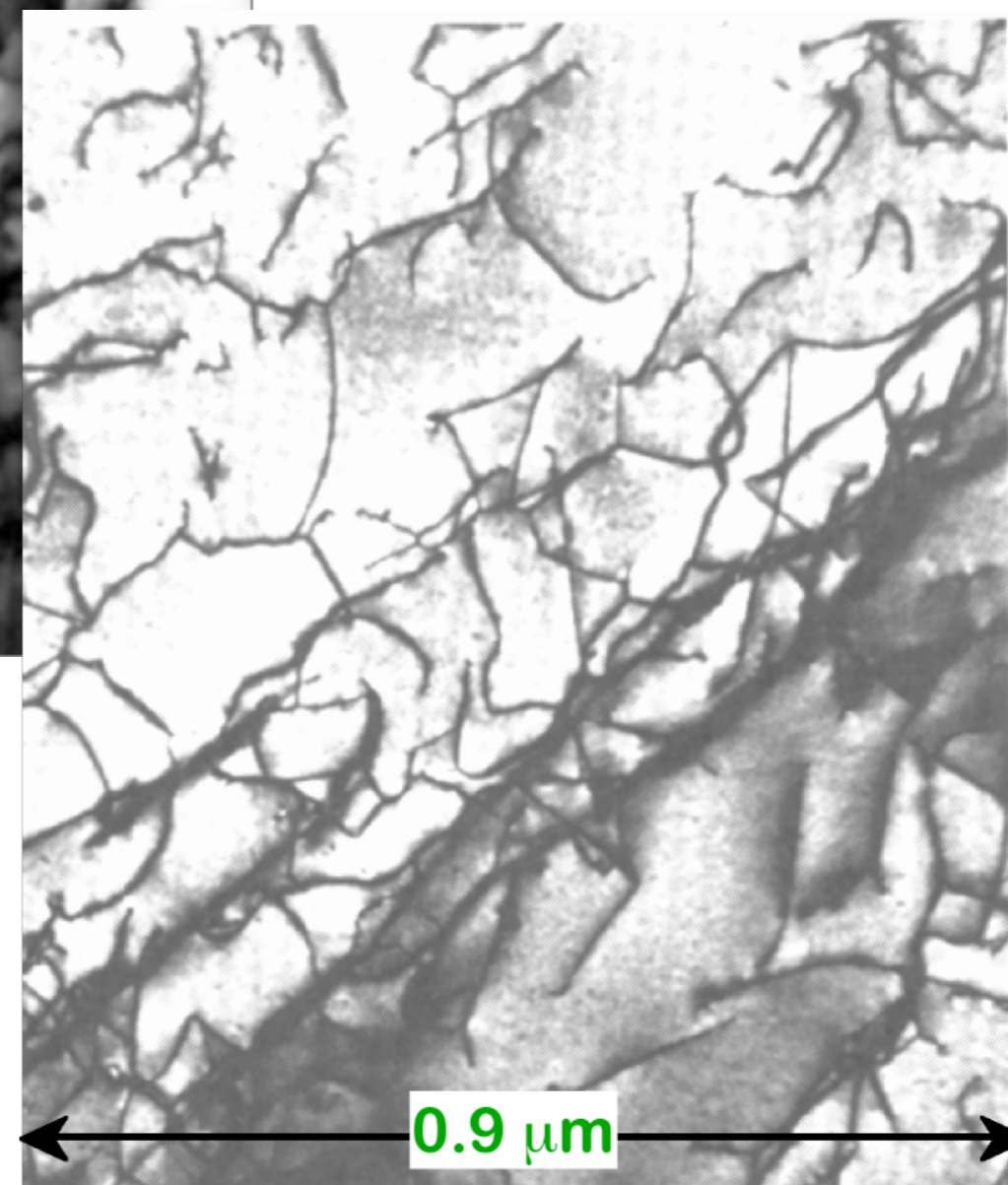
single x-tal Mo



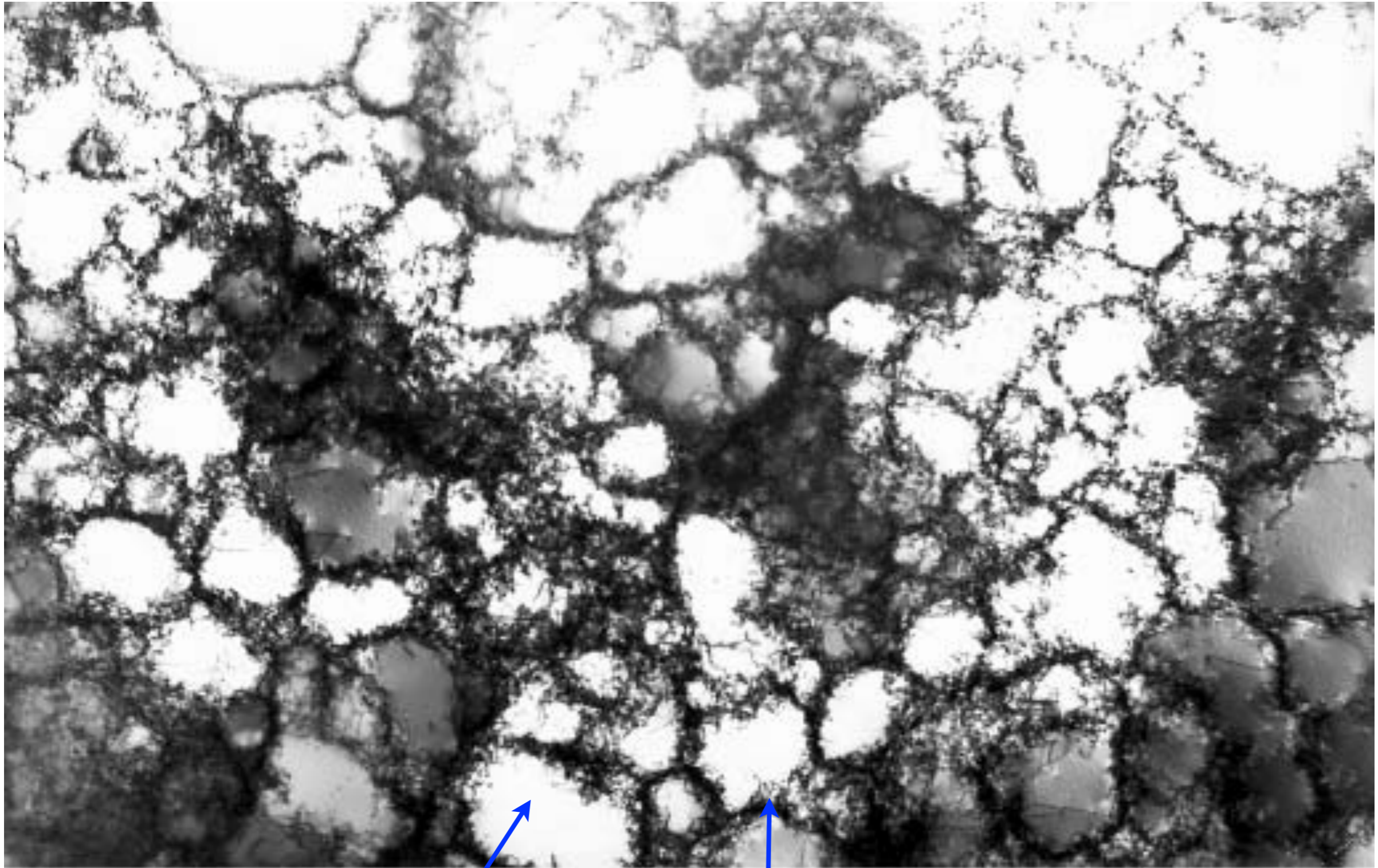
single x-tal Ni



Ti:



Stage III: Single crystal Cu [100] load



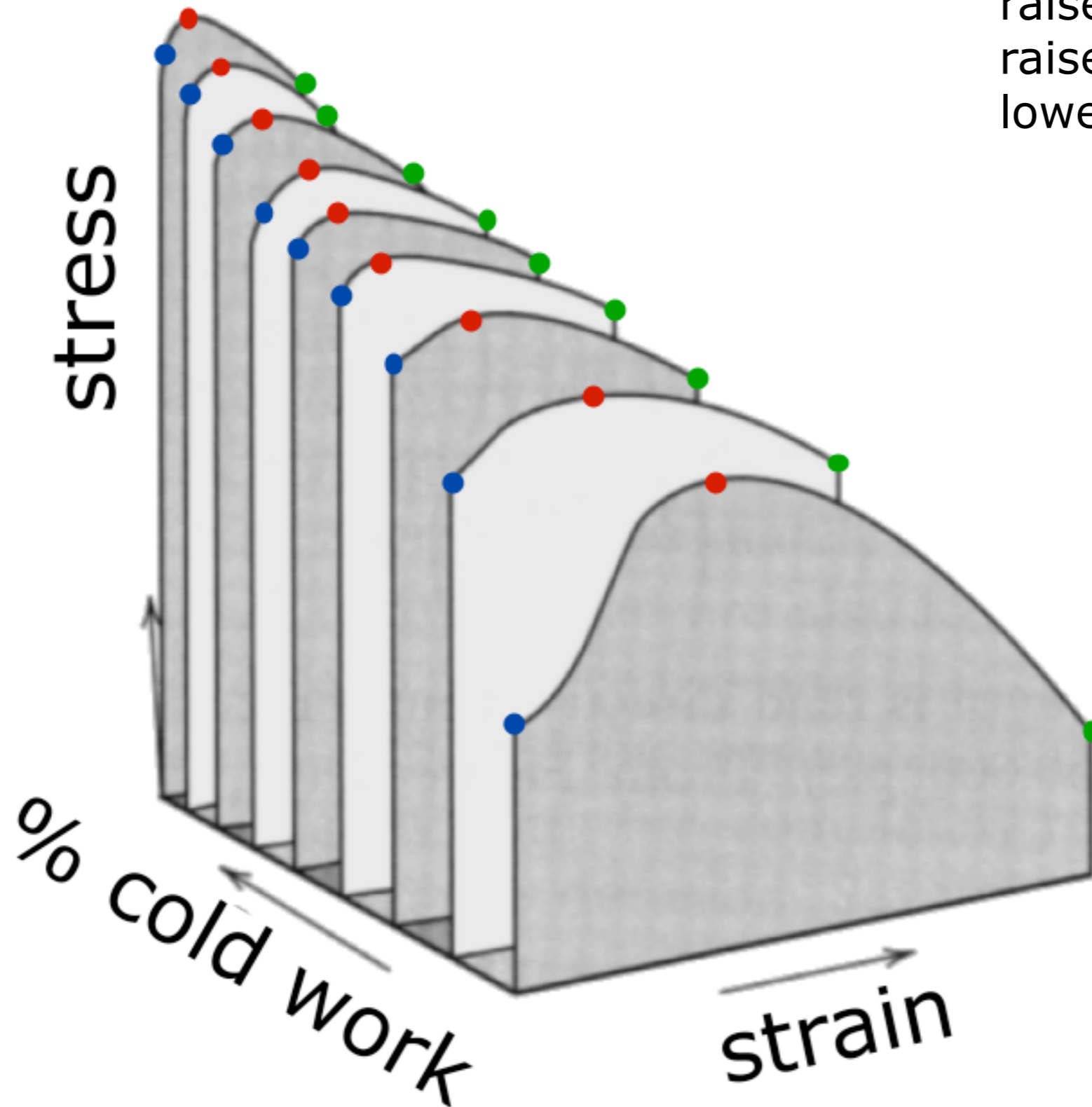
cell

dislocation wall

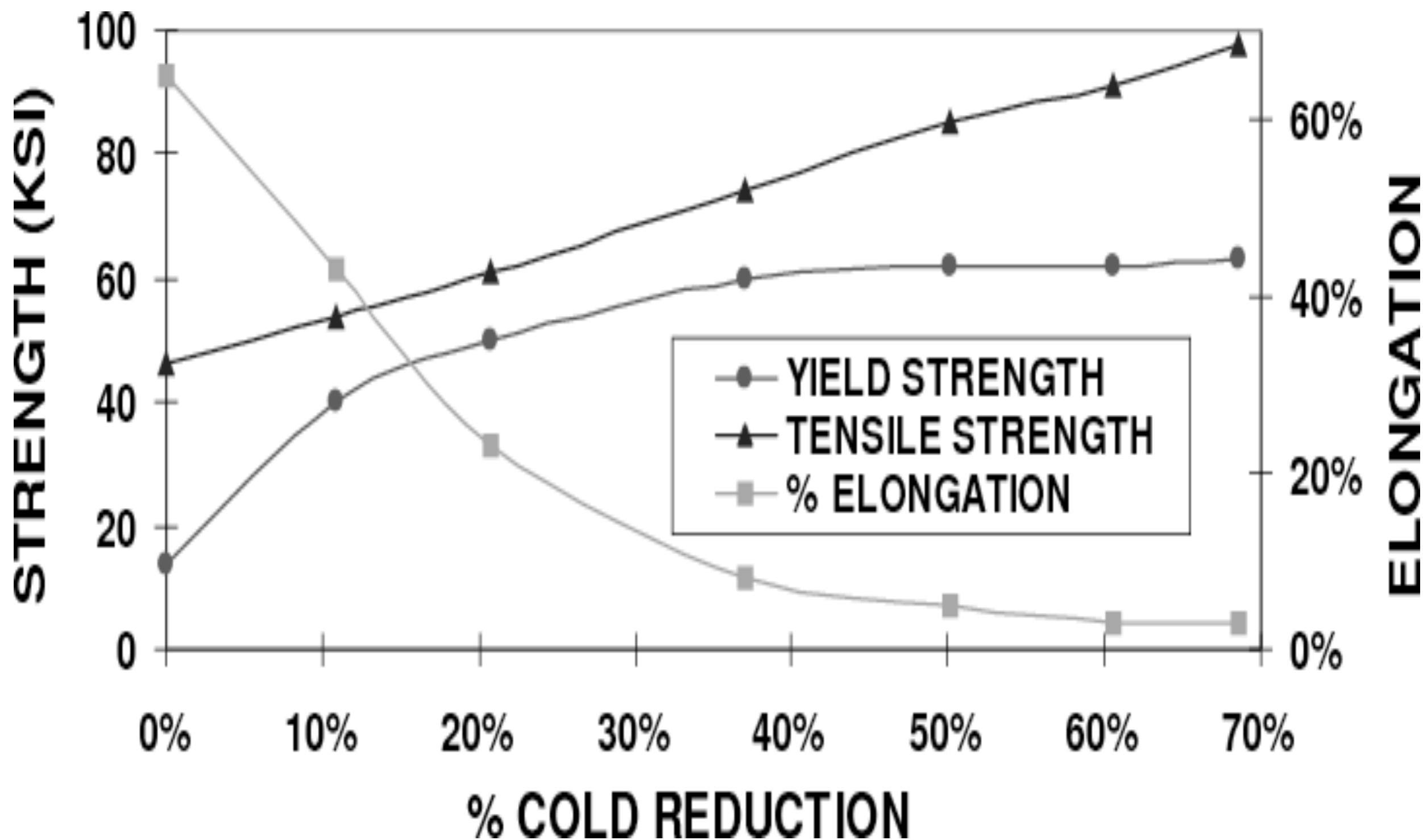
from H. Mughrabi

Effect of (repeated) cold-working

repeated wire-drawing:
raises yield stress
raises tensile stress
lowers ductility

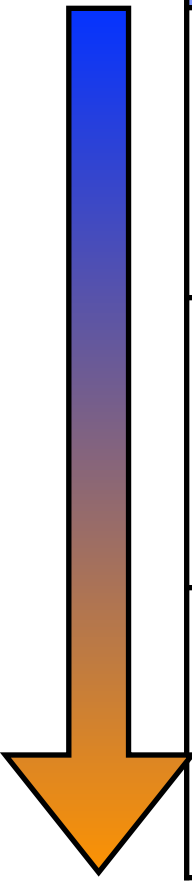


Effect of cold-working



Annealing stages

annealing stage	microstructural changes	dislocation density
recovery	strains relieved dislocation rearrange to reduce energy climb to form low-angle grain boundaries	slightly ↓
recrystallization	cold-work microstructure reduced strain-free grains nucleated	greatly ↓
grain growth	grain size increases reduction in grain boundary area	slightly ↓



increasing time/
temperature

Recrystallization: brass

33% cold-worked

3s anneal, 580°C



0.6mm

from Callister, 6nd edition

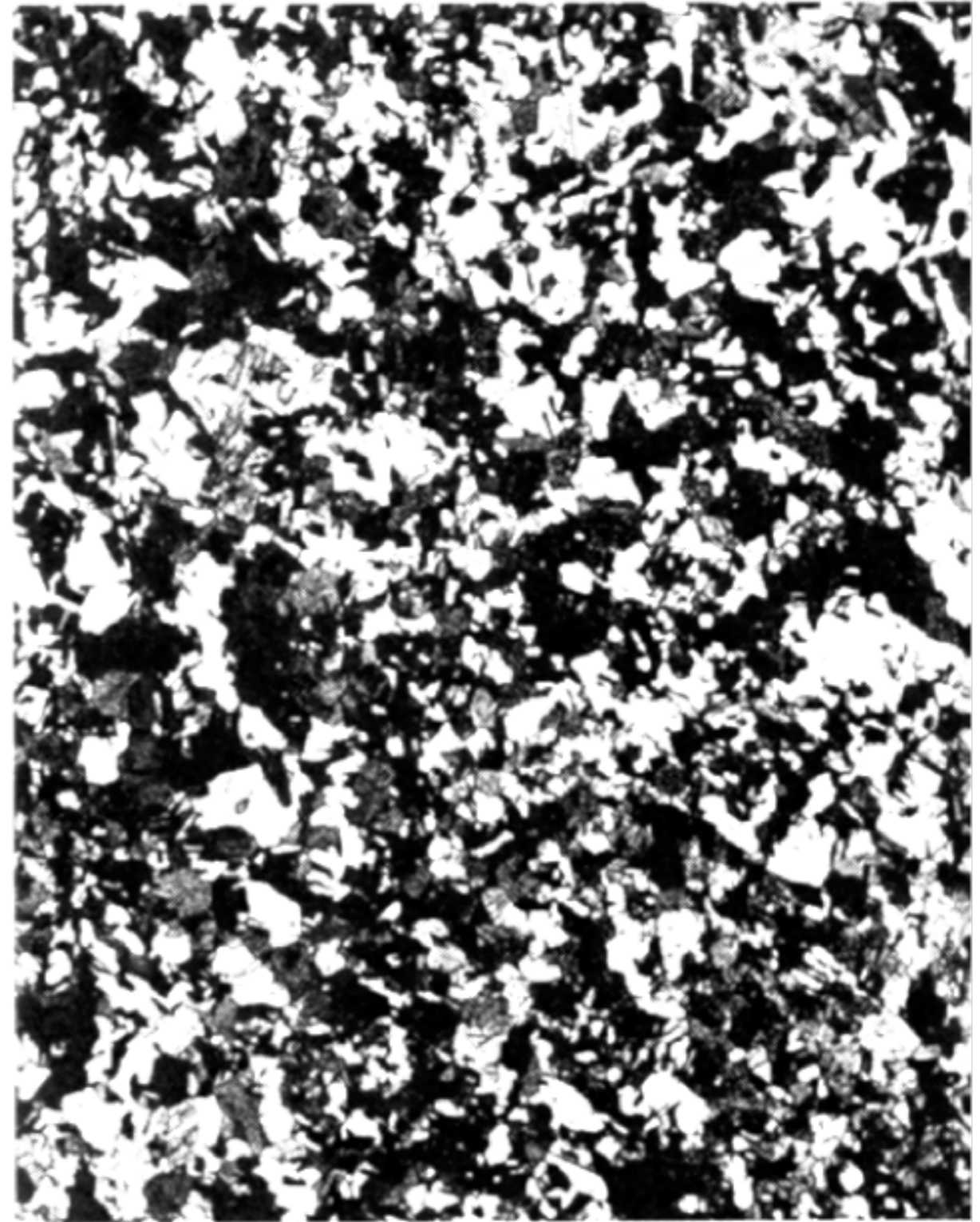
Recrystallization: brass, con't.

4s anneal, 580°C



0.6mm

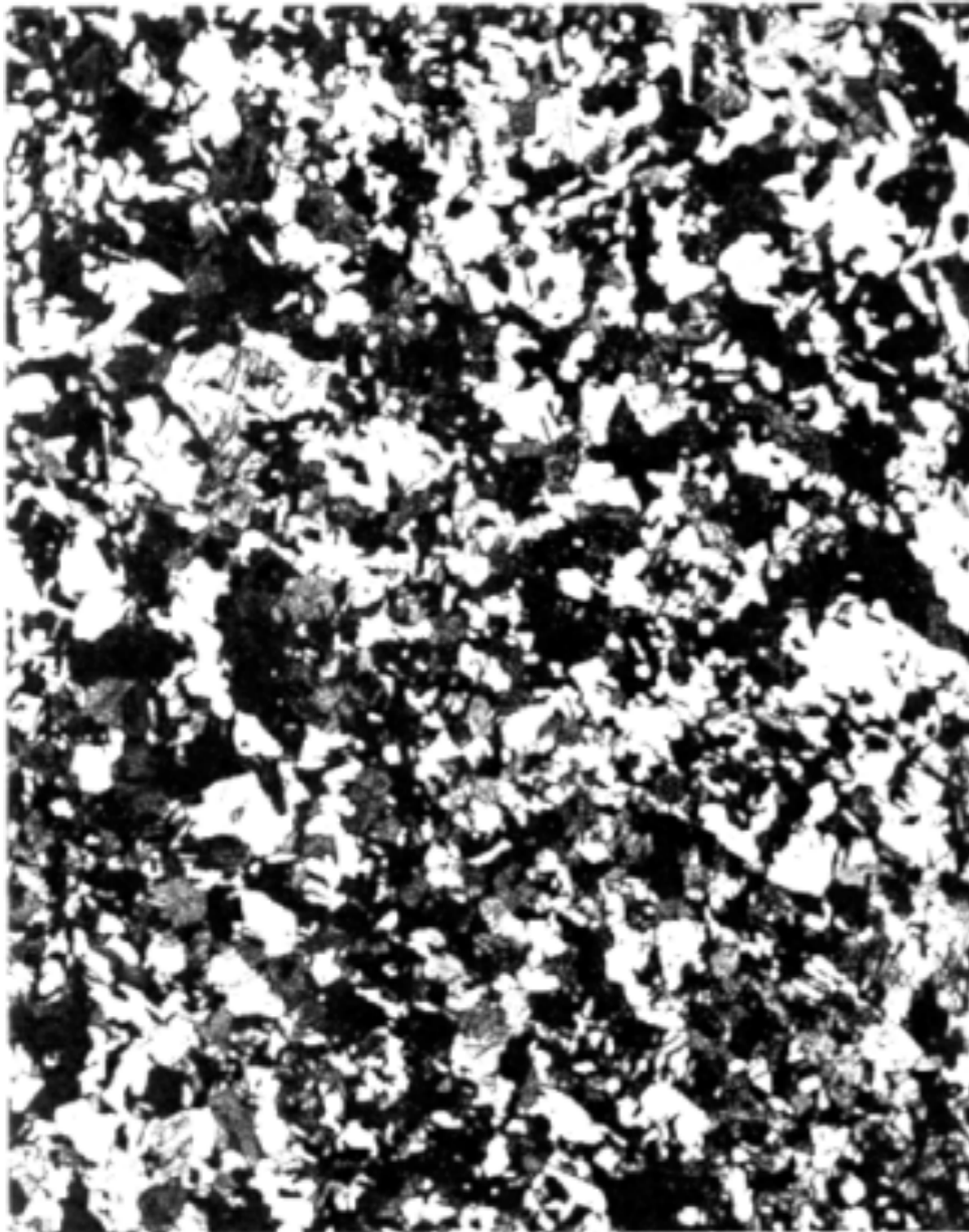
8s anneal, 580°C



from Callister, 6nd edition

Grain growth: brass

8s anneal, 580°C



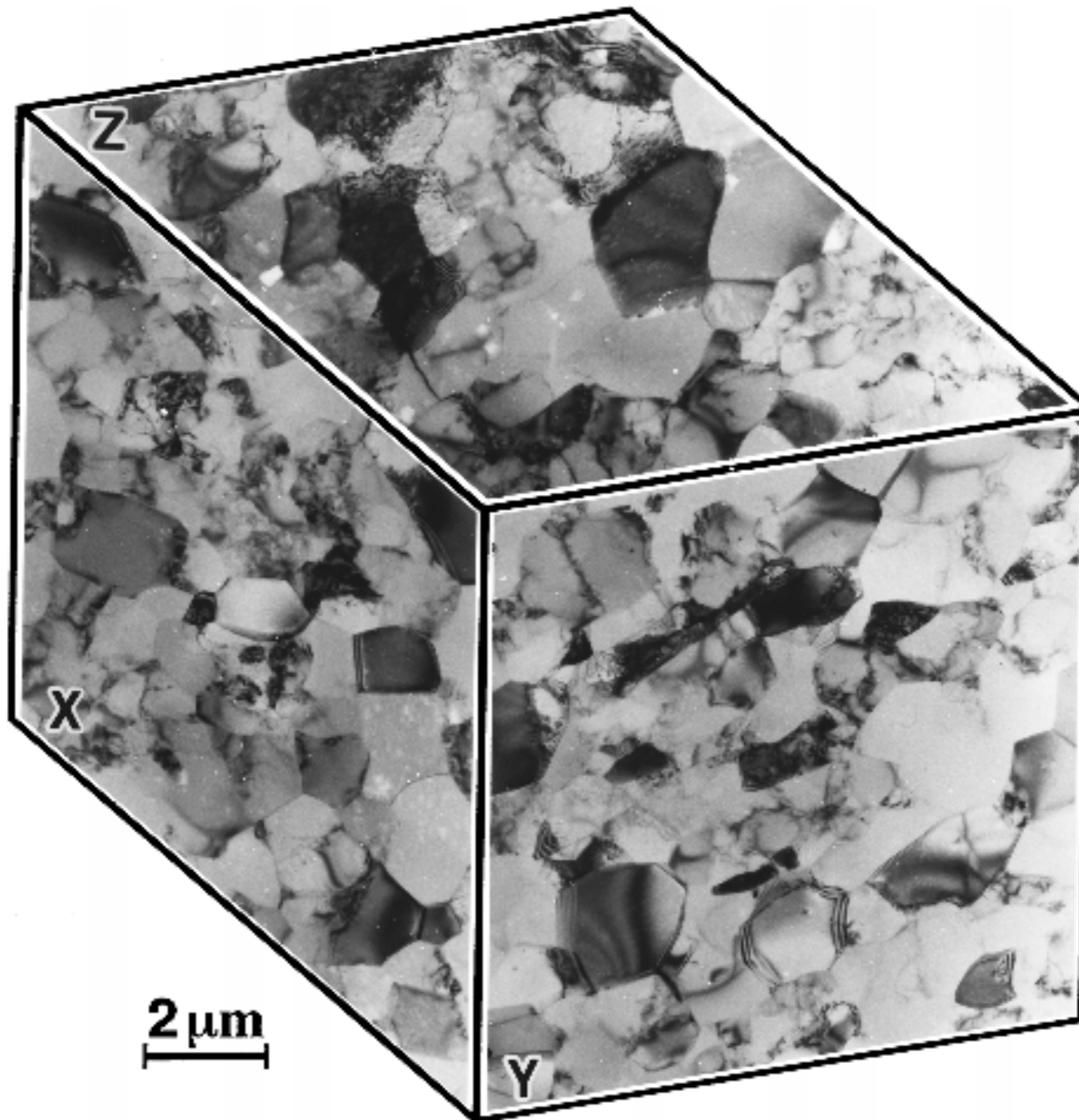
0.6mm

15min. anneal, 580°C



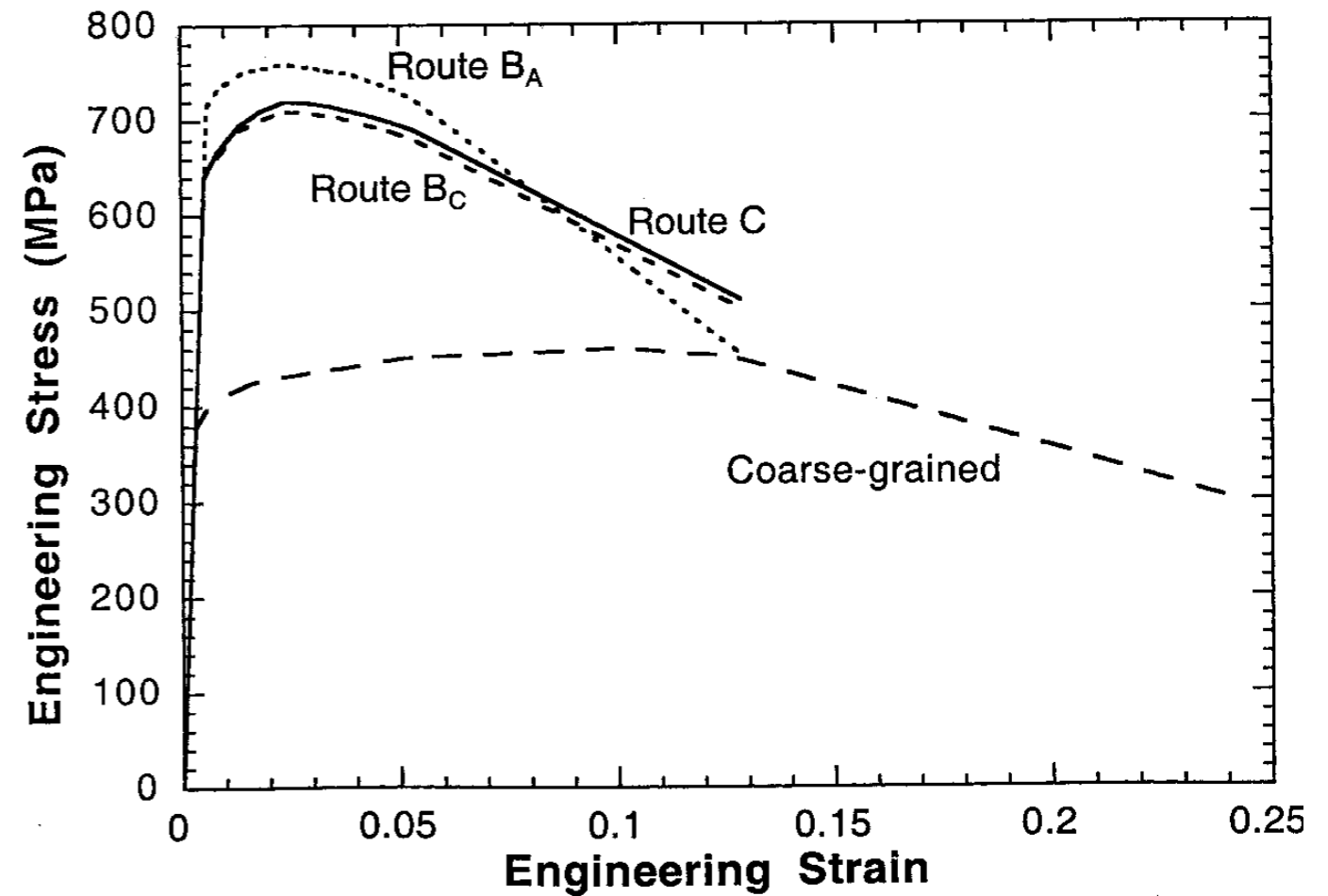
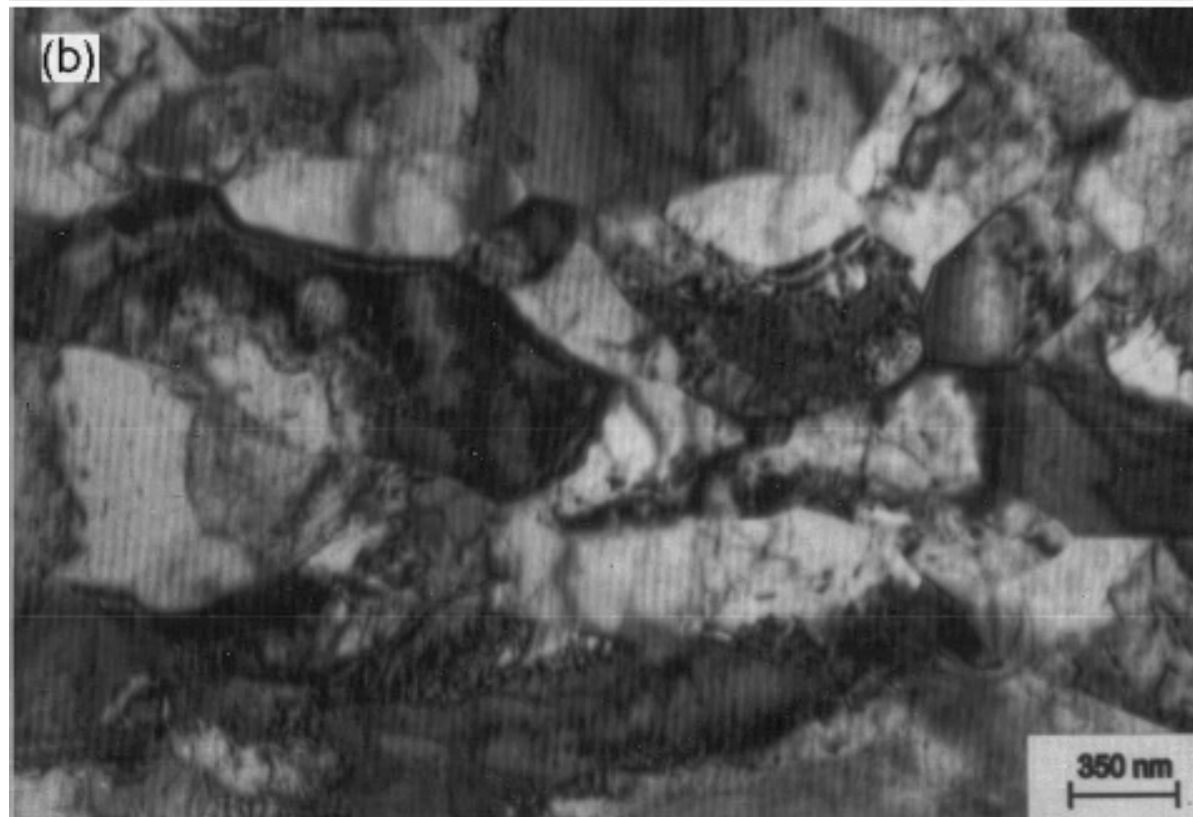
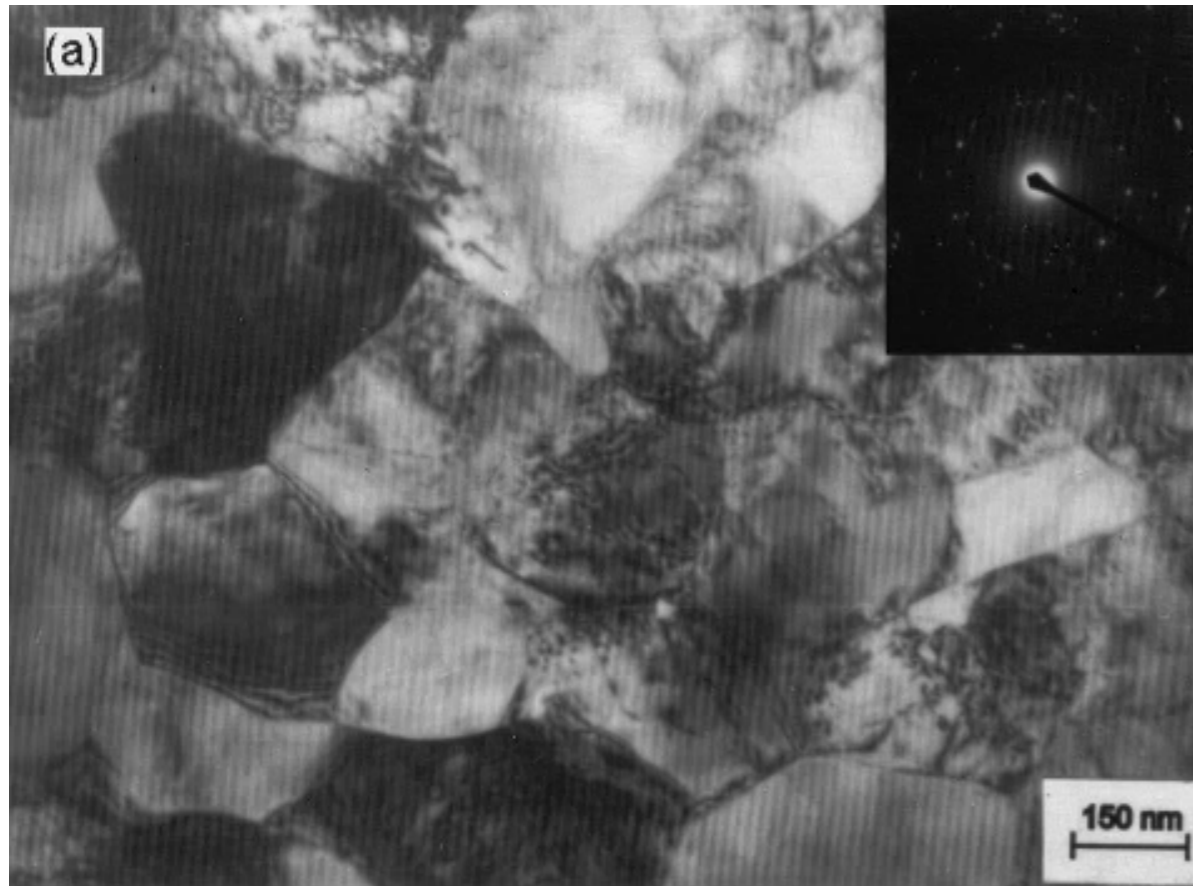
from Callister, 6nd edition

ECAP: Al microstructure



from M. Furukawa et al., J. Mater. Sci. **36**, 2835-2843 (2001)

ECAP Ti microstructure & properties



- Stress-strain test
- Necking, work-hardening, true stress/strain
- Multiaxial loading
- Crystal model of slip
- Topological defects
- Screw, edge, mixed
- Dislocation motion
- Peach-Koehler force
- Stress field of a dislocation
- Energy of a dislocation
- Dislocations in particular crystal structures: FCC, BCC, HCP, intermetallics
- Kinks and dislocation mobility
- Dislocation intersections and jogs
- Relationship between dislocation motion and plasticity
- Solute-dislocation interactions
- Solid solution strengthening
- Dislocations as obstacles
- Work-hardening stages

Dislocations and plastic deformation

