DEFECTS IN CRYSTALS: DISLOCATIONS, INTERFACES AND GRAIN BOUNDARIES

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OUTLINE

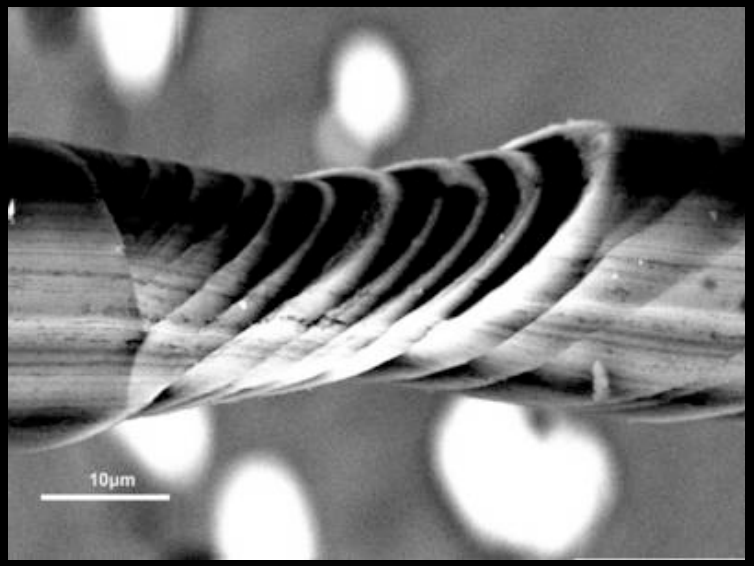
- Lecture 1: Dislocations
- Lecture 2: Planar defects: Interfaces, grain boundaries
- Lecture 3: Interfacial energy, interfacial stress
- Lecture 4: Phase field crystal method: continuum method for defect formation and evolution

REFERENCES: DISLOCATIONS

- Shewmon: Transformations in Metals
- Weertman and Weertman: Elementary Dislocation Theory
- Hull and Bacon: Introduction to Dislocations
- Theory of Dislocations: Hirth and Lothe

DISLOCATIONS

- Hypothesized in the 1930's by Polyani, Orowan and Taylor to account for the very low yield stress of metals



Single Crystal Aluminum

http://physnano.univie.ac.at/typo3temp/pics/0f853d7432.jpeg

table 1-1 *Critical resolved shear stress for single crystals.*

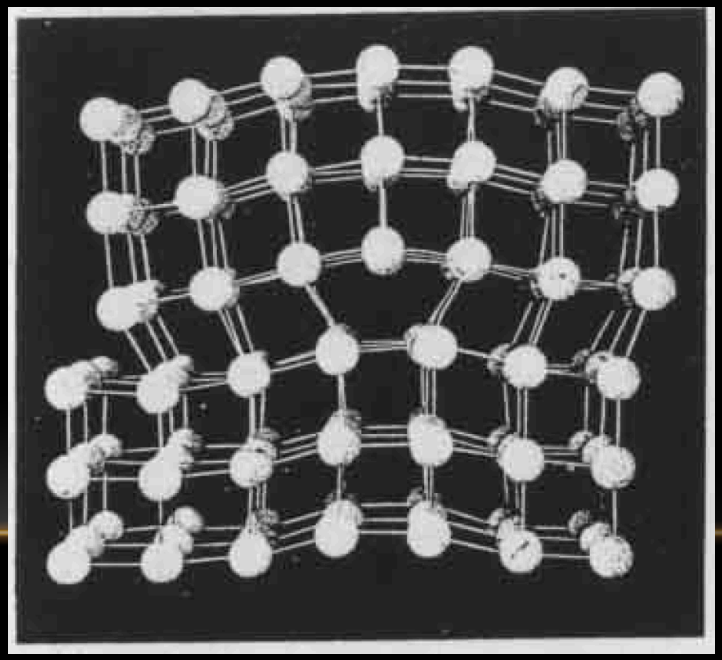
Metal	*Structure*	*G, psi*	*CRSS, psi**
Al	fcc	3.9×10^6	148
Cu	fcc	7.0×10^6	92
Mg	hcp	2.4×10^6	63
Zn	hcp	5.6×10^6	26
α-Fe	bcc	9×10^6	4,000

* R. Read-Hill, "Physics of Metals Principles," chap. 4, D. Van Nostrand Company, Inc., Princeton, N.J., 1964.

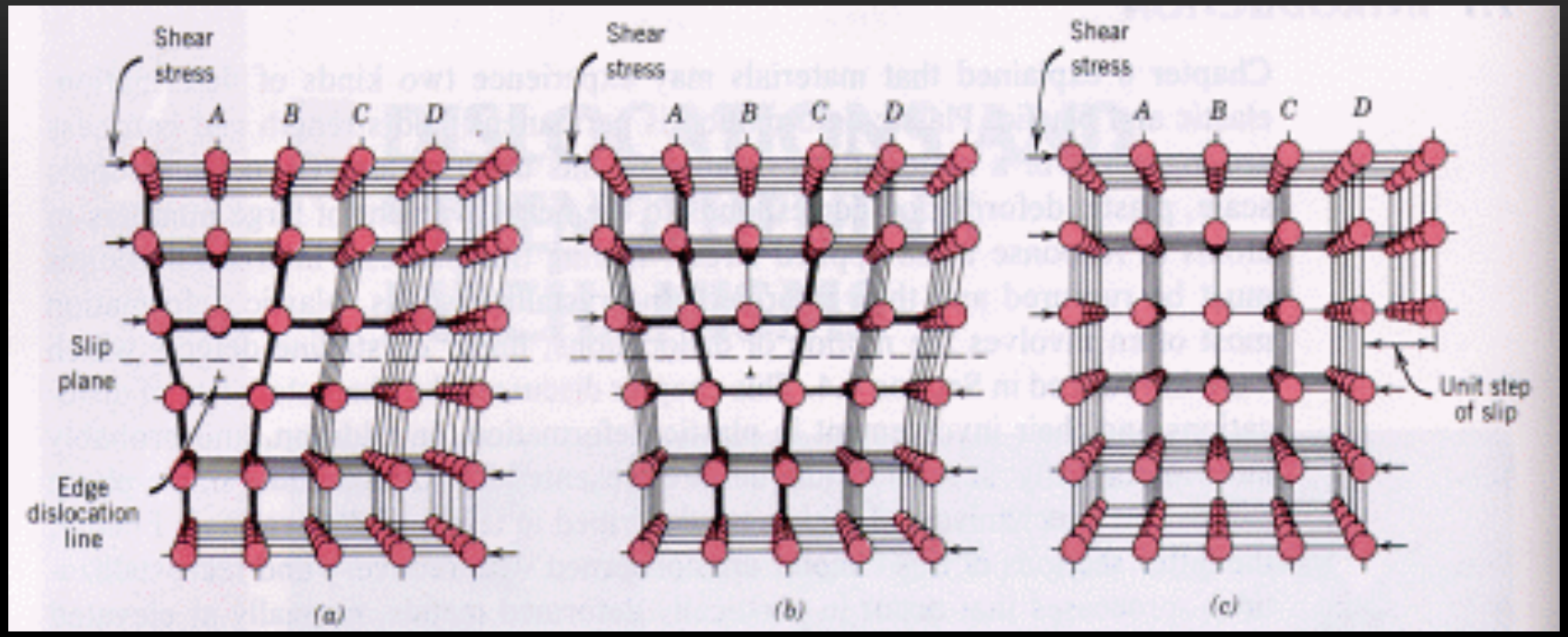
- 148 Psi implies that a 0.5 in diameter rod of Al will deform under a load of only 30 pounds
- By contrast the stress required to move one layer of atoms over another is on the order of G/6
- Answer: need a mechanism that allows only one atom plane to move at a time. These are dislocations.

DISLOCATIONS

- Line defects that demark the deformed from undeformed region of a crystal
- Simple examples: edge dislocations and screw dislocations
- Edge dislocation:

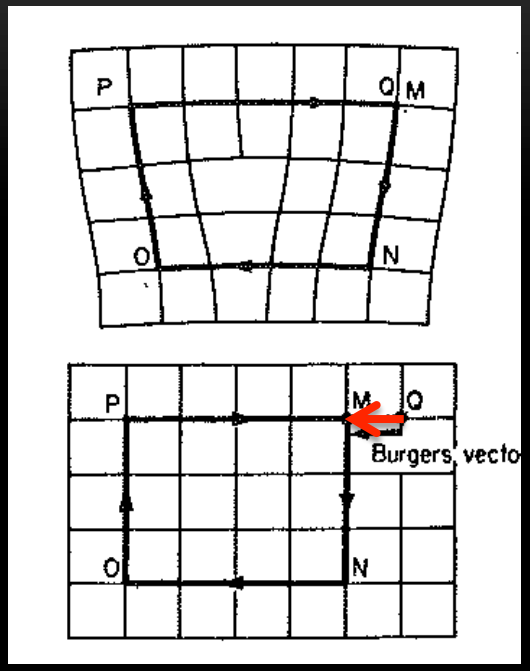


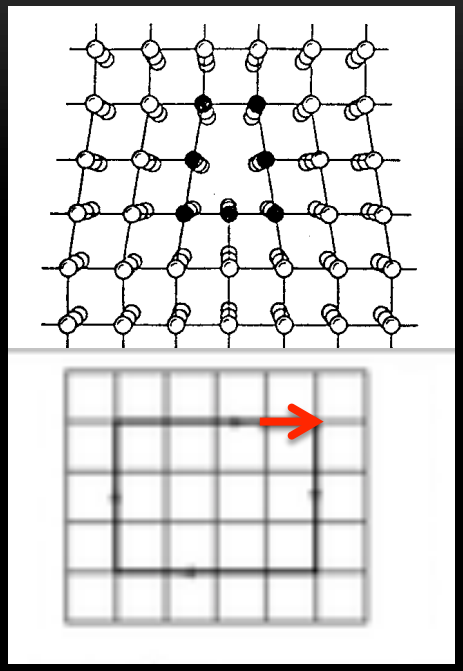
Edge dislocation motion:



- For each atom moved from its equilibrium location, there is an atom that is moved towards its equilibrium location
- Amount of displacement is the Burgers vector b
- Dislocation line vector ξ, thus $\mathbf{b} \bullet \xi = 0$
- Dislocation moves in the direction of b

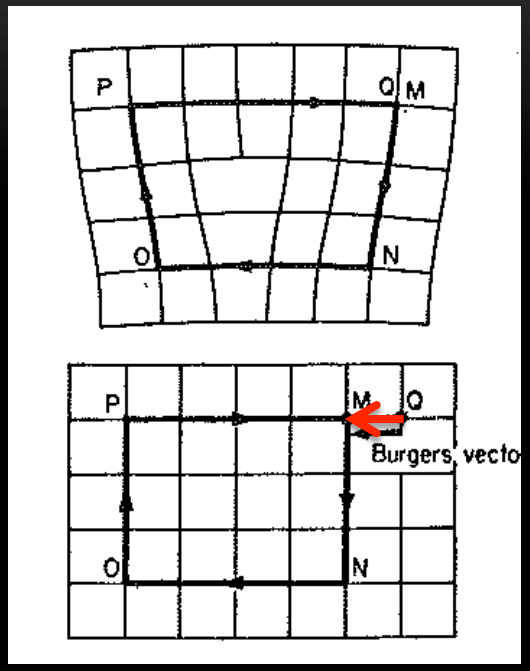
Defining a Burgers vector: edge dislocation

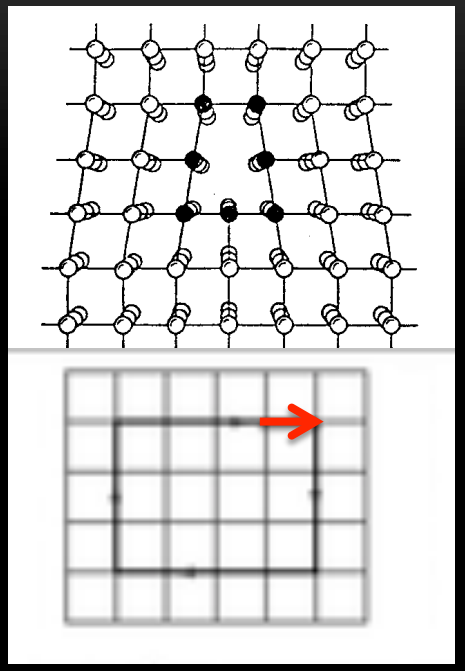




- Define a line direction, move around in the dislocation, count the number of planes
- Repeat in a perfect crystal
- Connect the end to the start: Right hand, finish start
- Arbitrary, but once fixed do not change: positive and negative b
- Depends on the direction along which the dislocation is viewed

Defining a Burgers vector: edge dislocation





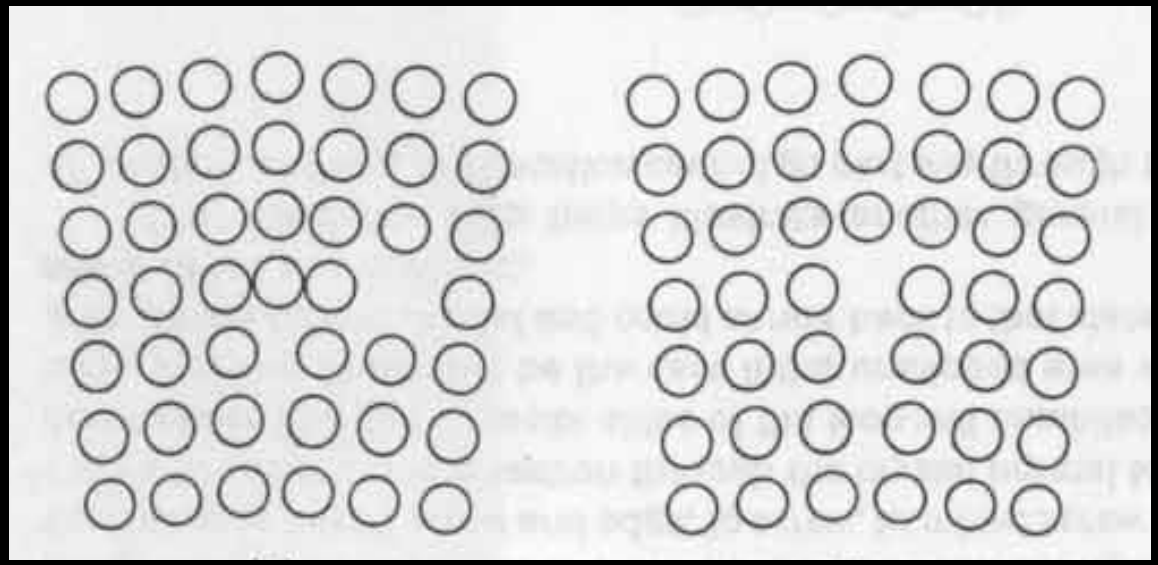
- Well defined slip plane:

$$\mathbf{n} = \mathbf{b} \times \xi$$

- In the absence of climb, edge dislocations are constrained to move a plane

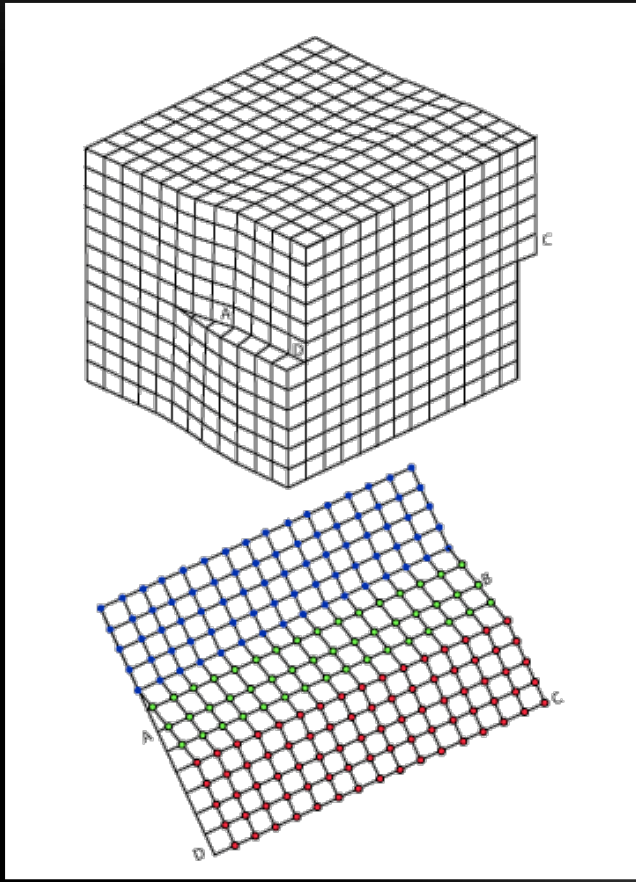
DISLOCATION CLIMB

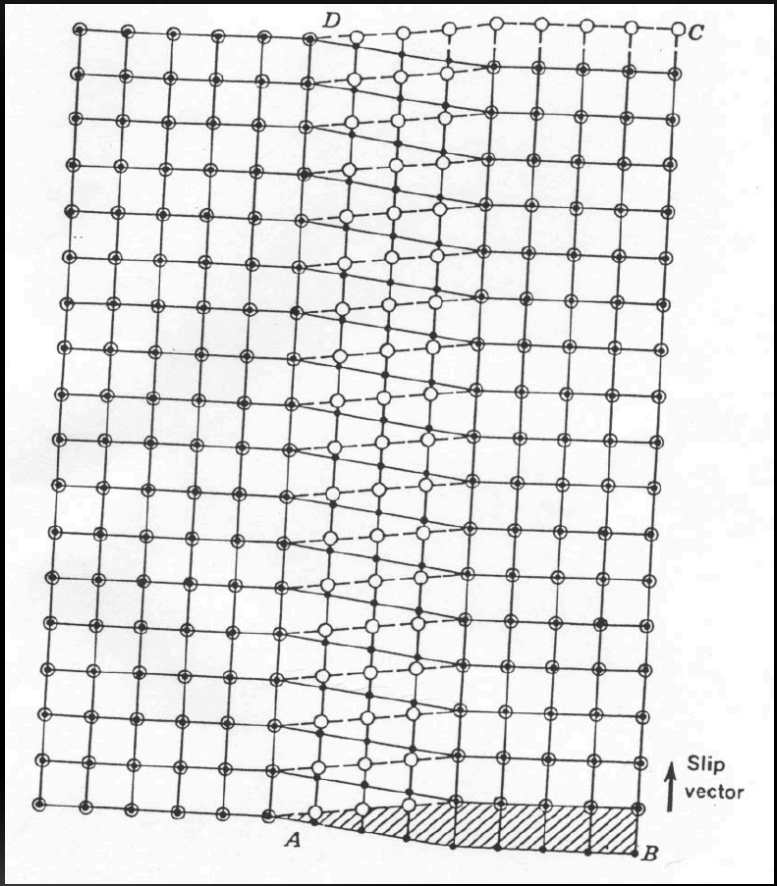
- Dislocations can be sources of vacancies



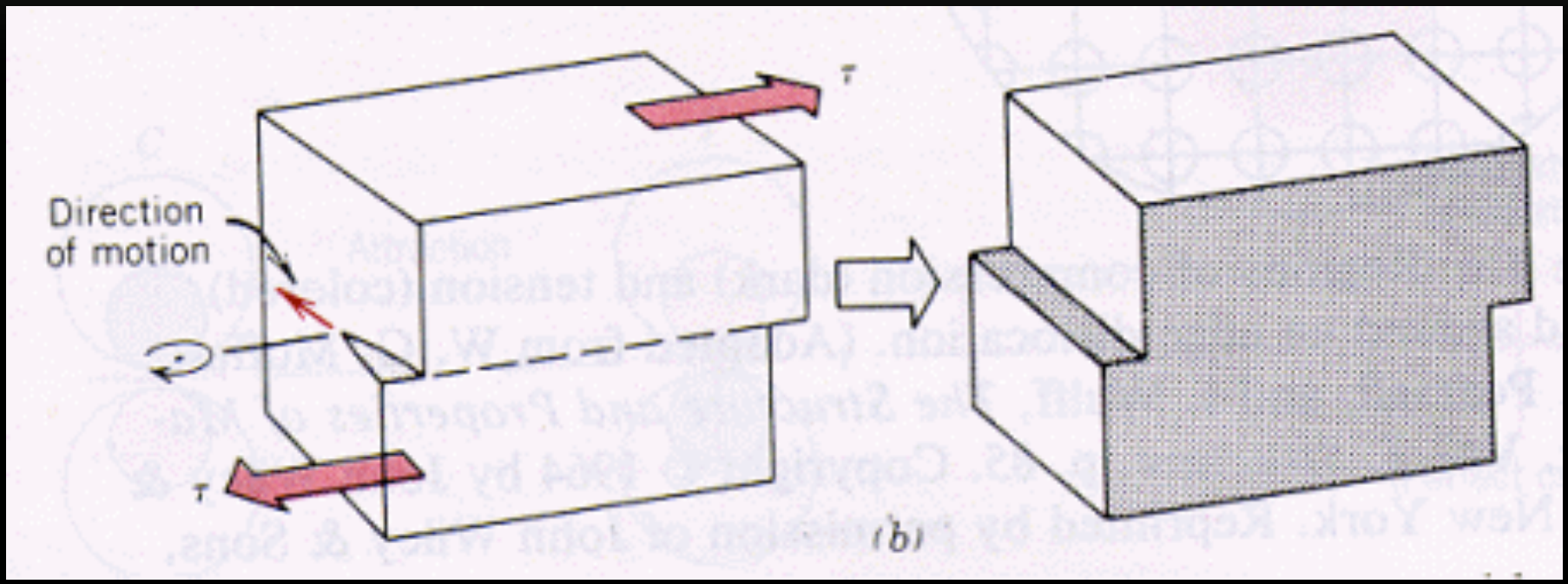
- Thus materials can creep and vacancies are not conserved in crystals with high dislocation densities

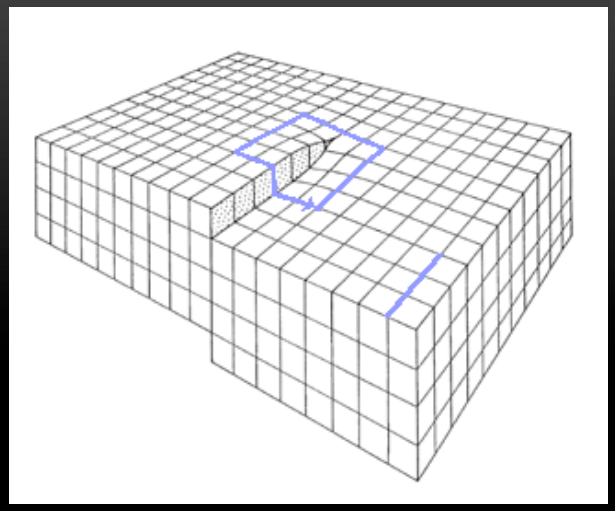
SCREW DISLOCATIONS

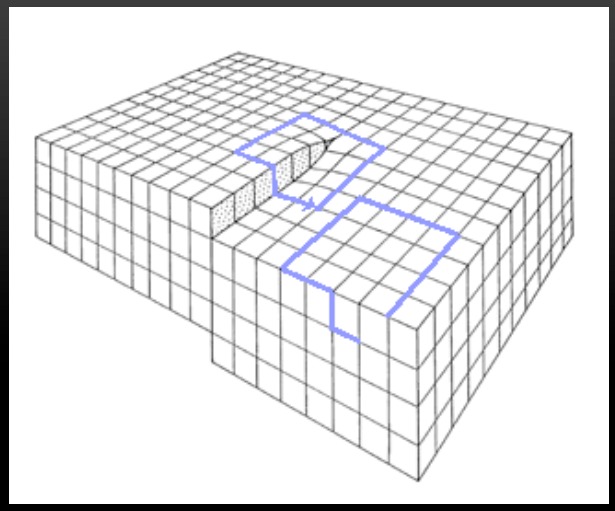




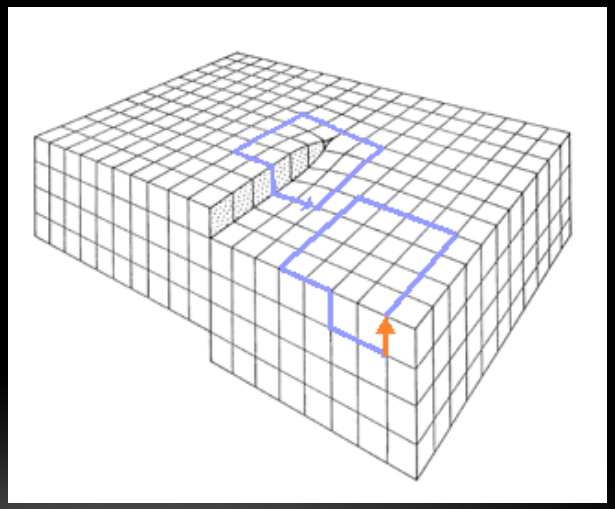
SCREW DISLOCATION MOTION







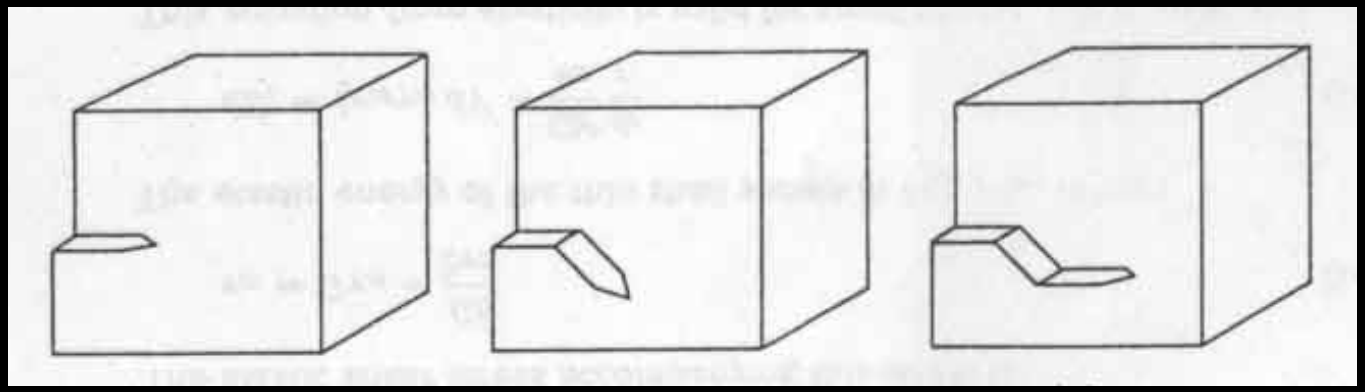
$\mathbf{b} \parallel \xi$

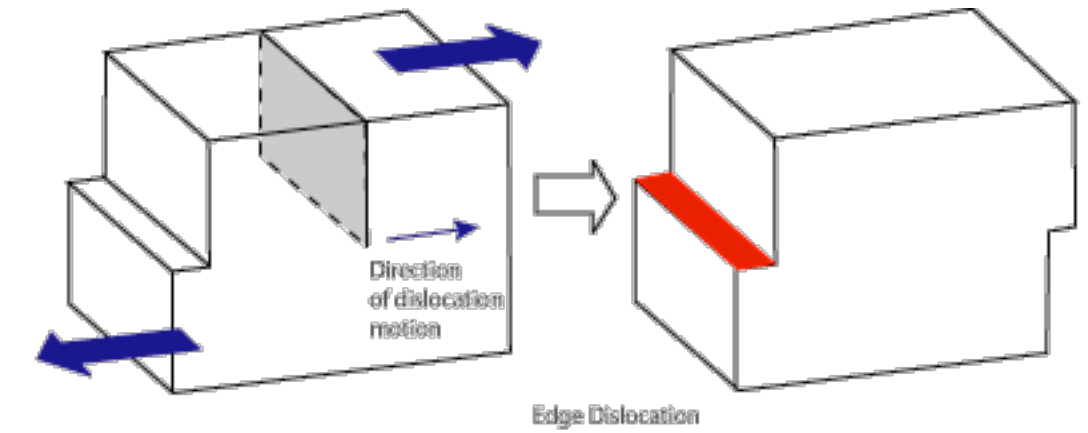


http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/illustr/511burg2.gif

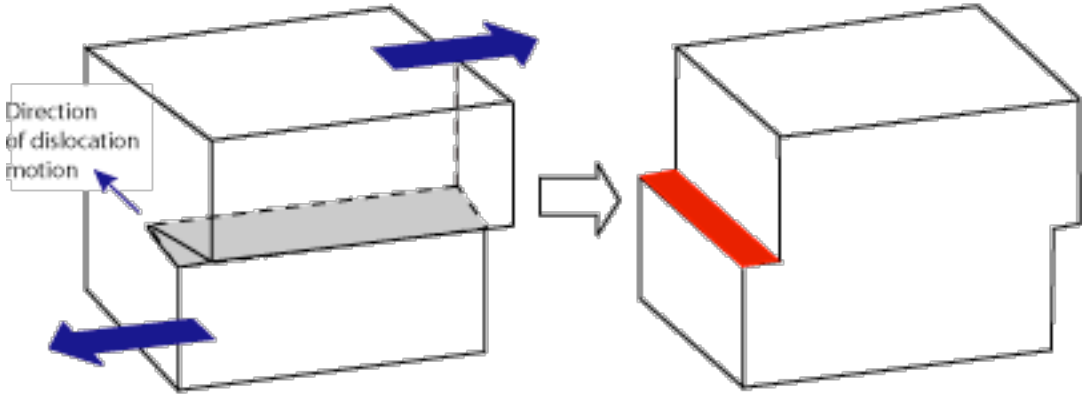
CROSS SLIP

- Screw dislocations do not have a well defined slip plane (absent crystallography!)
- Cross slip is possible:



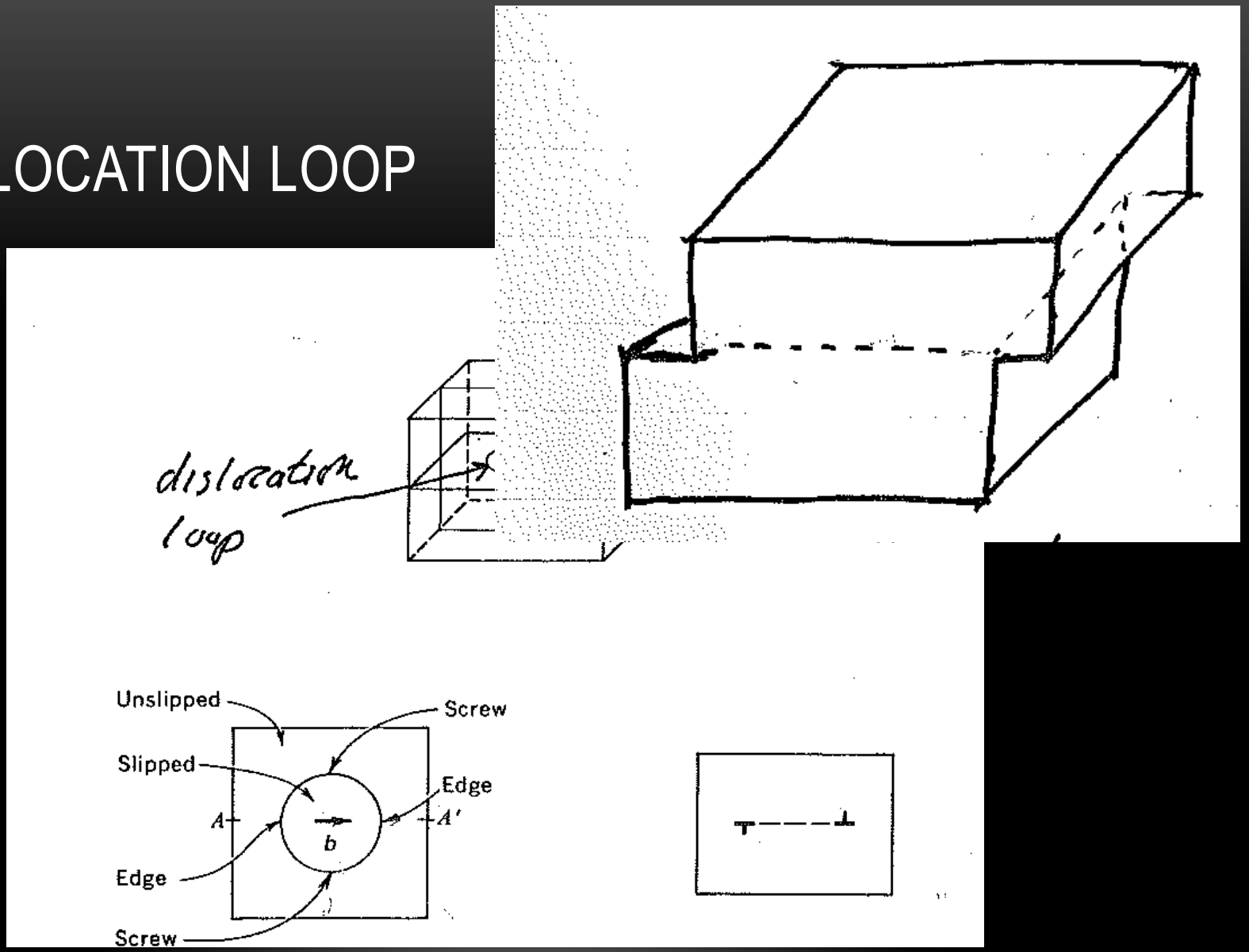


Edge Dislocation



Screw Dislocation

DISLOCATION LOOP



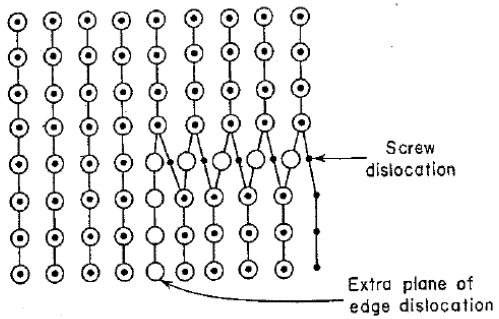


Fig. 4.17 Atomic configuration corresponding to the dislocation of Fig. 4.16 viewed from above. Open-circle atoms above slip plane, dot atoms below slip plane.

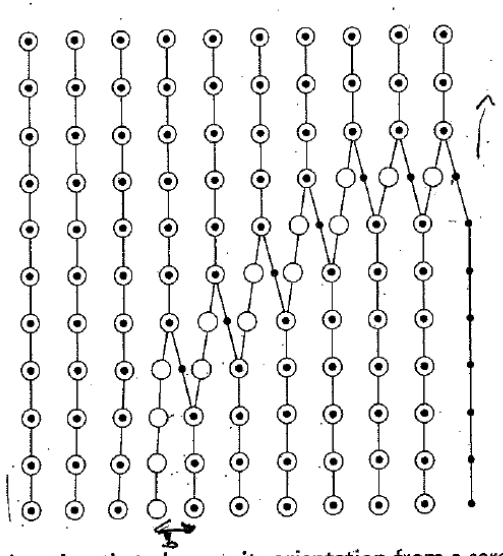
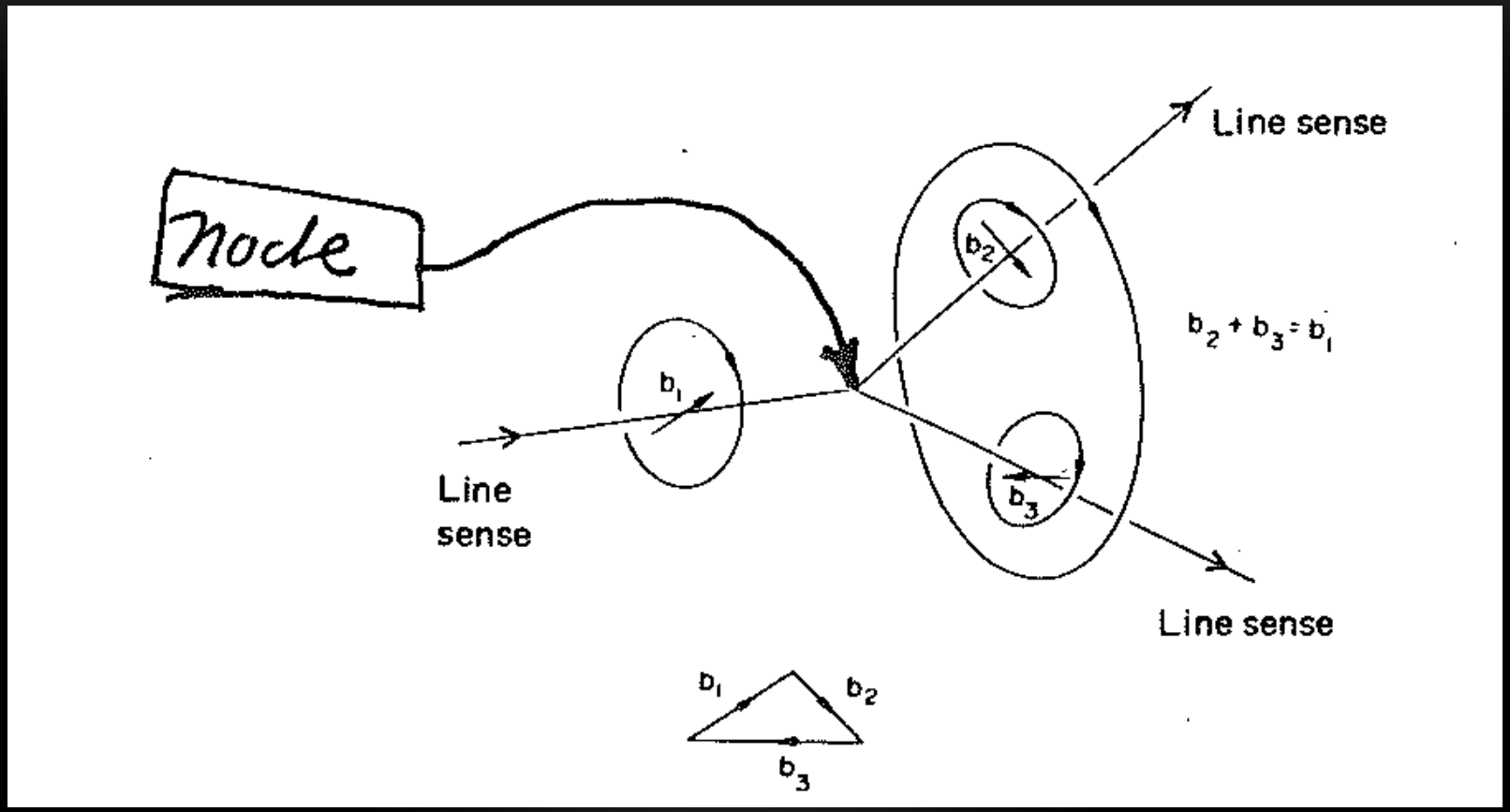


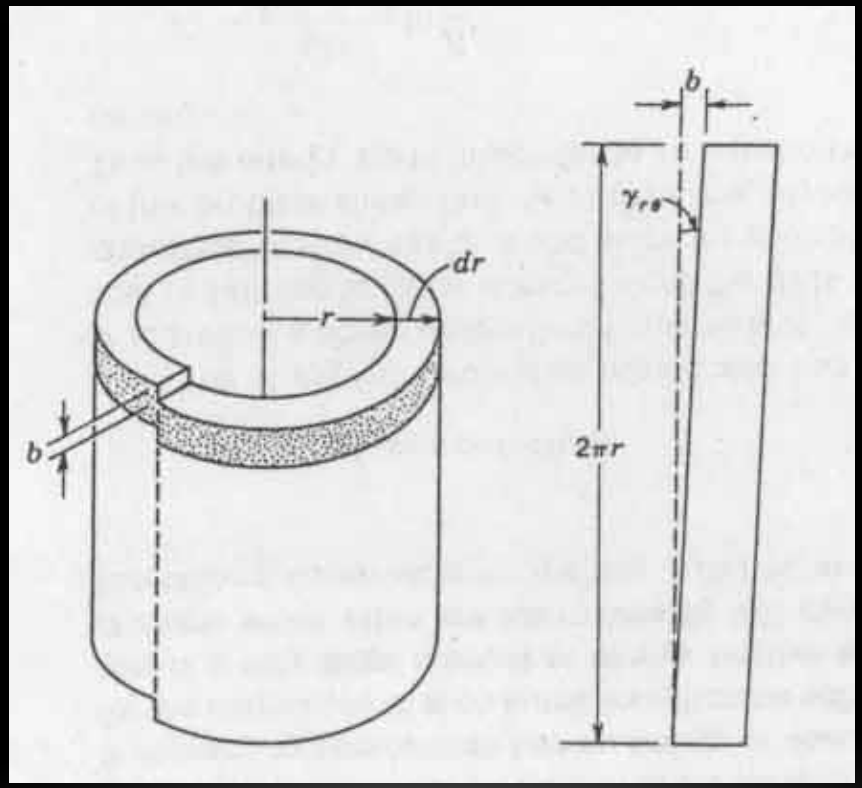
Fig. 4.18 A dislocation that changes its orientation from a screw to an edge as viewed from above looking down on its slip plane.

Dislocations cannot end in a crystal



ELASTIC FIELD INDUCED BY A SCREW DISLOCATION

Linear isotropic elasticity



$$u_z = b\frac{\theta}{2\pi}$$

$$\epsilon_{\theta z} = \frac{b}{2\pi r}$$

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

ELASTIC FIELD DUE TO A SCREW DISLOCATION

- Long ranged stress field
- Pure shear
- Strain energy:

$$E_v \sim \sigma\epsilon \sim 1/r^2$$

$$E_l = \frac{\mu b^2}{4\pi}\int_0^\infty \frac{1}{r}dr$$

- Divergence at infinity: answer depends on sample size
- Divergence at 0: failure of linear elasticity

ELASTIC FIELD DUE TO A DISLOCATION

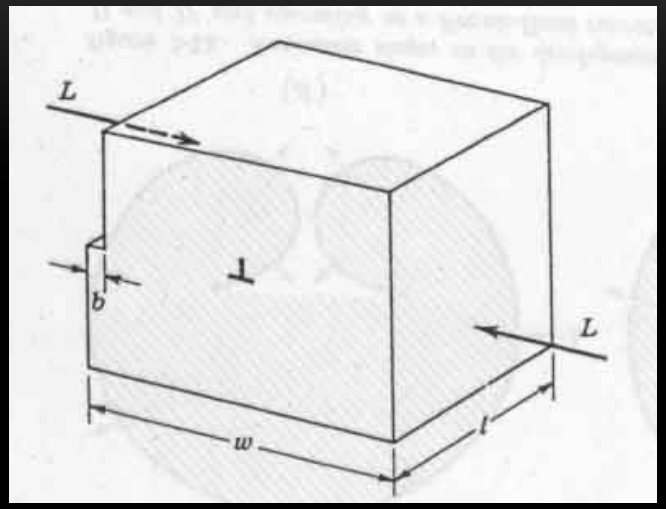
- Defining a core radius below which linear elasticity does not hold:

$$E_l = \frac{\mu b^2}{4\pi} \ln \frac{r}{r_o}$$

- Energy is proportional to b^2
- Energy is proportional to the line length: dislocation loops will contract
- Energy varies weakly with location
- Energy of an edge dislocation differs by only an order 1 constant

FORCE ACTING ON A STRAIGHT DISLOCATION

$$\tau = \frac{L}{wl}$$



Total work done by the external load must equal that required to move the dislocation a distance w:

$$Lb = F_s w$$

$$\frac{F_s}{l} = \tau b$$

GENERALIZATION: PEACH-KOEHLER FORCE

$$\frac{F_s}{l} = \tau b$$

$$\frac{F_g}{l} = \frac{[(\mathbf{b} \cdot \sigma) \times \xi] \cdot [\xi \times (\mathbf{b} \times \xi)]}{|\mathbf{b} \times \xi|}$$

INTERACTIONS BETWEEN DISLOCATIONS

- Two straight, parallel screw dislocations on the same slip plane, same sign of b,

$$F_s' = \tau b = \frac{\mu b^2}{2\pi r}$$

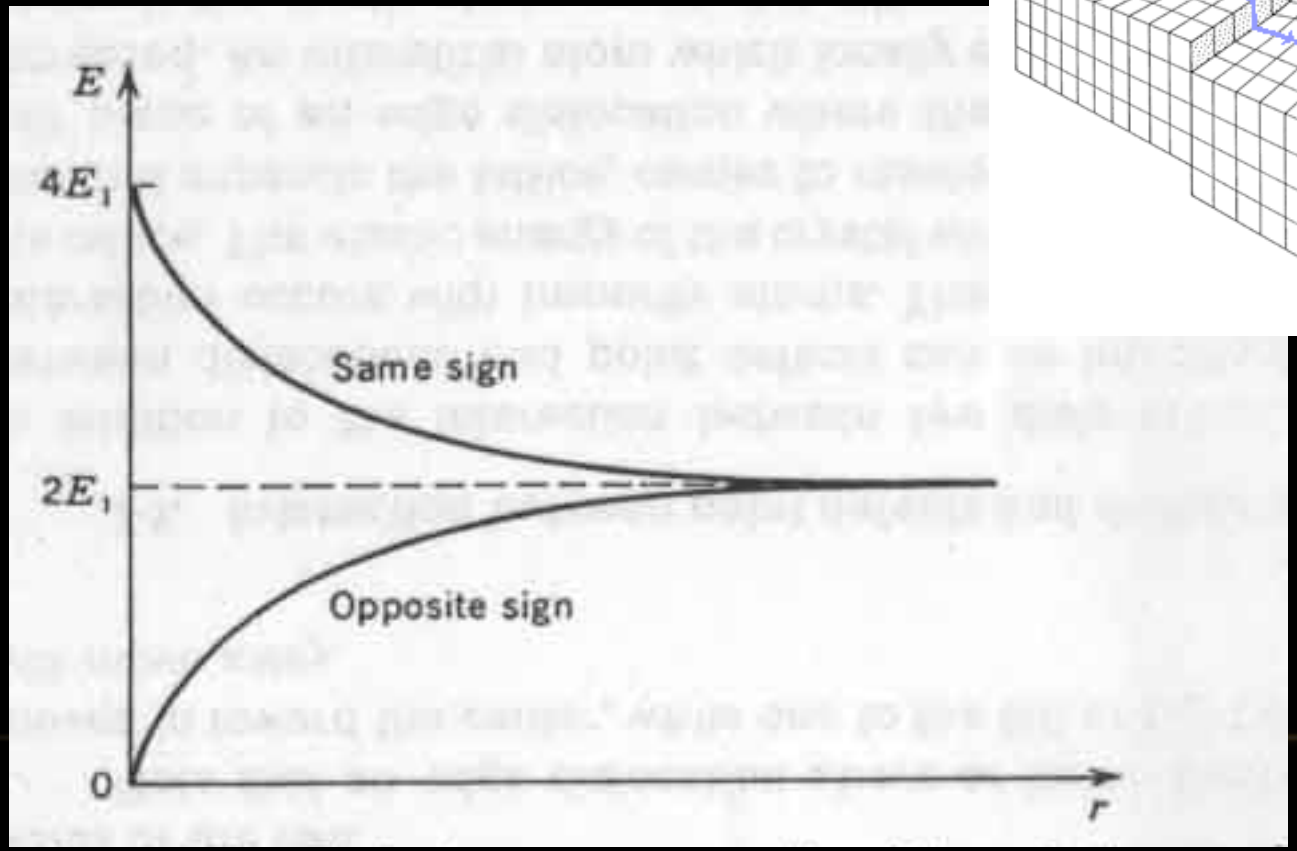
- Force is repulsive, along the normal to the line
- If b are of different sign,

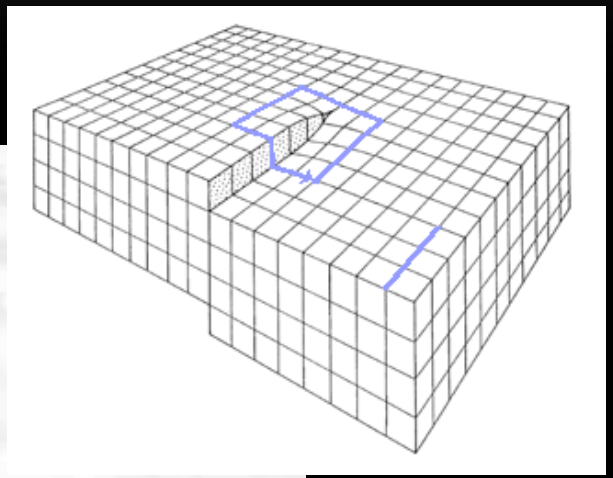
$$F_s' = \tau b = -\frac{\mu b^2}{2\pi r}$$

- The force is attractive

INTERACTION ENERGY BETWEEN TWO SCREW DISLOCATIONS

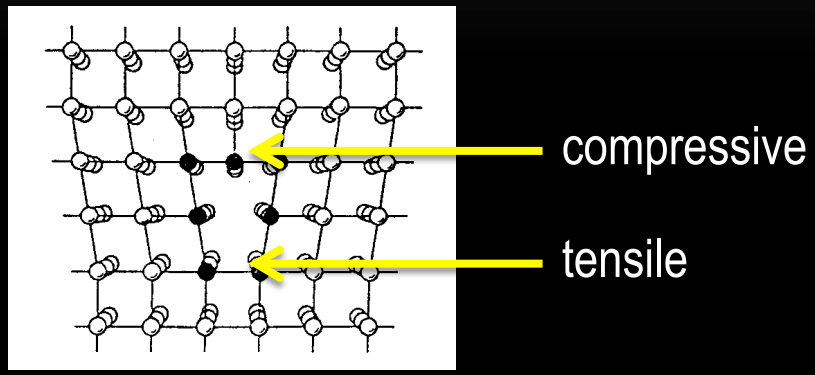
$$F_s' = \tau b = \frac{\mu b^2}{2\pi r} \qquad E_s = \frac{\mu b^2}{4\pi} \ln(r/r_o)$$



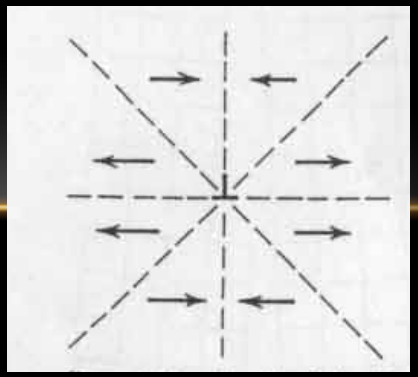


INTERACTIONS BETWEEN DISLOCATIONS

- The situation is more complicated for edge dislocations



- Along the slip plane, the results are identical with screw dislocations
- If the two edge dislocations are not on the same slip plane, then they can repel or attract:



STRESS REQUIRED TO EXPAND A DISLOCATION LOOP

- The energy change on expanding a loop is

$$2\pi T \delta R$$

  where T is the line tension (energy/length)

- Energy change due to force per length acting on the dislocation loop is

$$-2\pi R F_s' \delta R$$

- At equilibrium these sum to zero,

$$\left(2\pi T - 2\pi R F_s'\right) \delta R = 0$$

STRESS REQUIRED TO EXPAND A DISLOCATION LOOP

- Since,

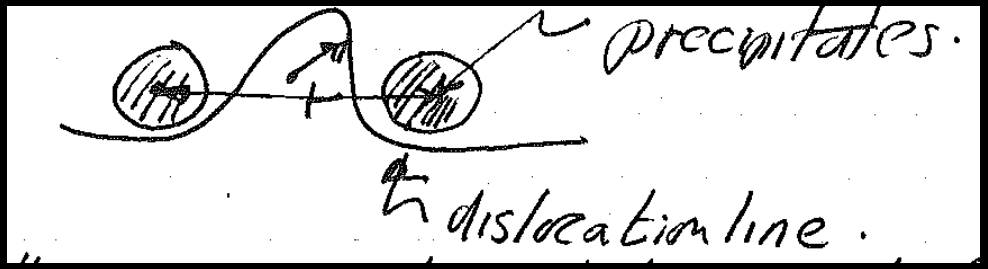
$$\frac{F_s}{l} = F_s' = \tau b$$

- The equilibrium condition is,

$$\tau = \frac{T}{Rb}$$

APPLICATIONS OF EQUILIBRIUM CONDITION

- Strengthening of alloy due to precipitations: Orowan



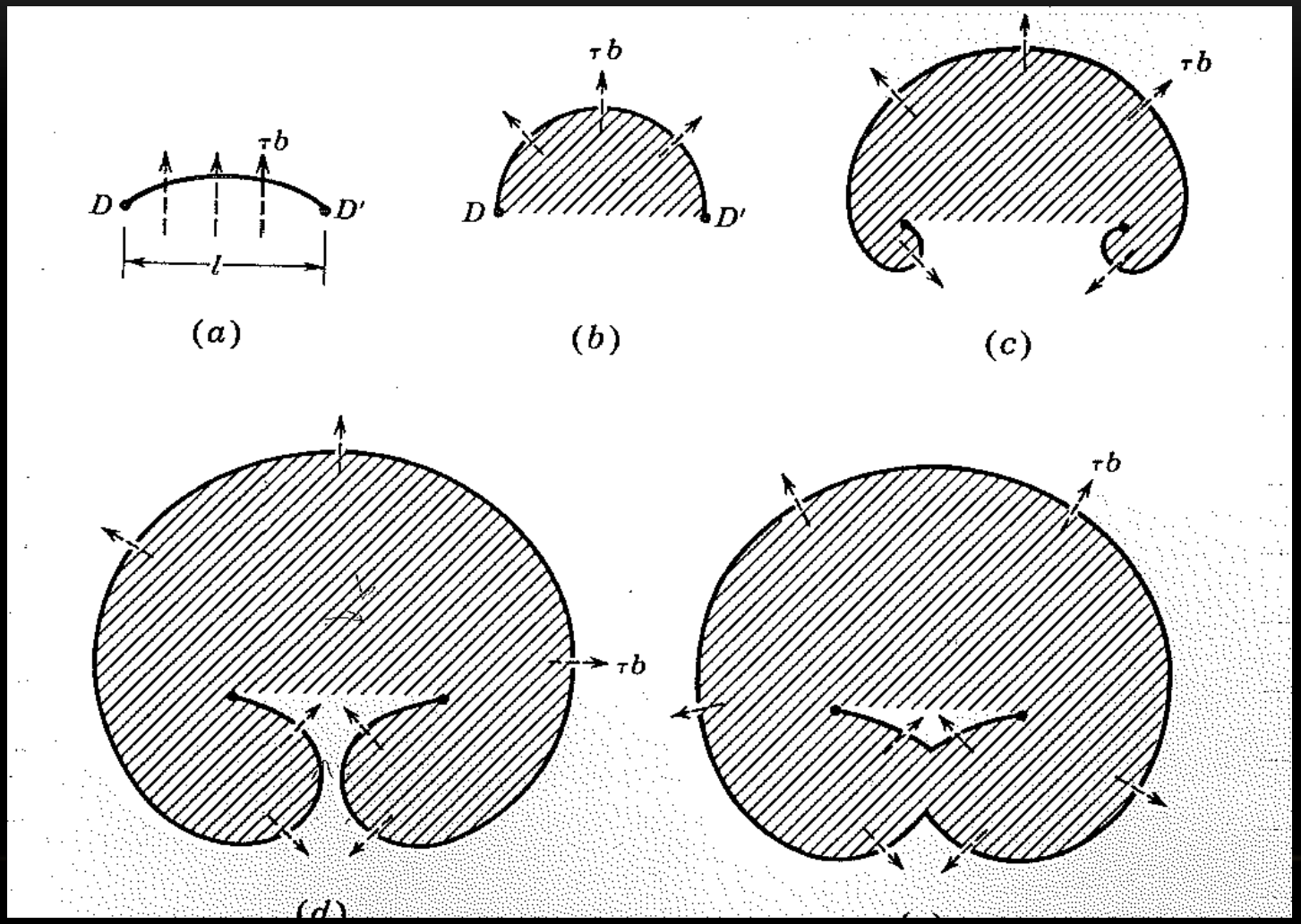
$$\tau = \frac{T}{Rb}$$

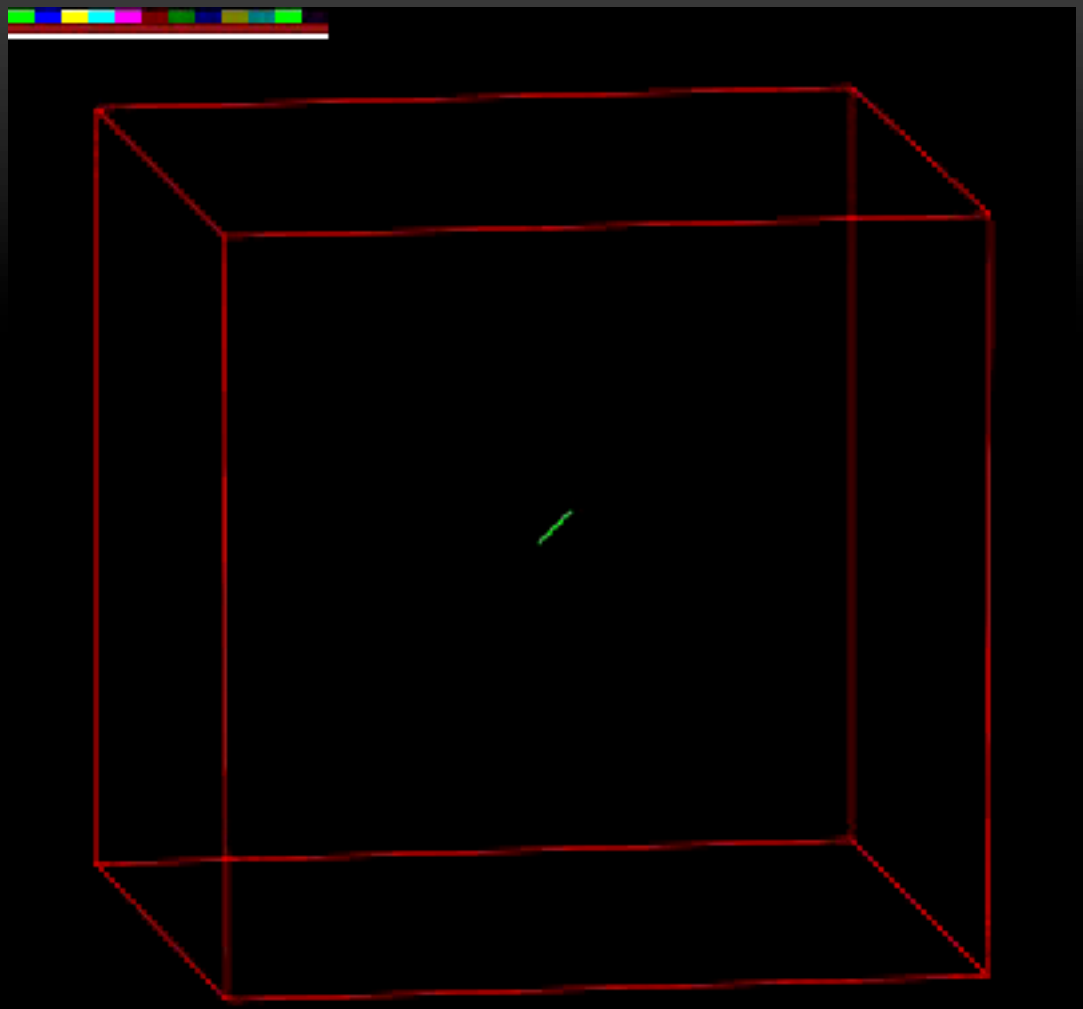
The distance between precipitates determines the yield strength of an alloy

- Problem: dislocation density of a solidified metal is way too low to account for the observed deformation

FRANK-READ SOURCE

$$\tau = \frac{T}{Rb}$$





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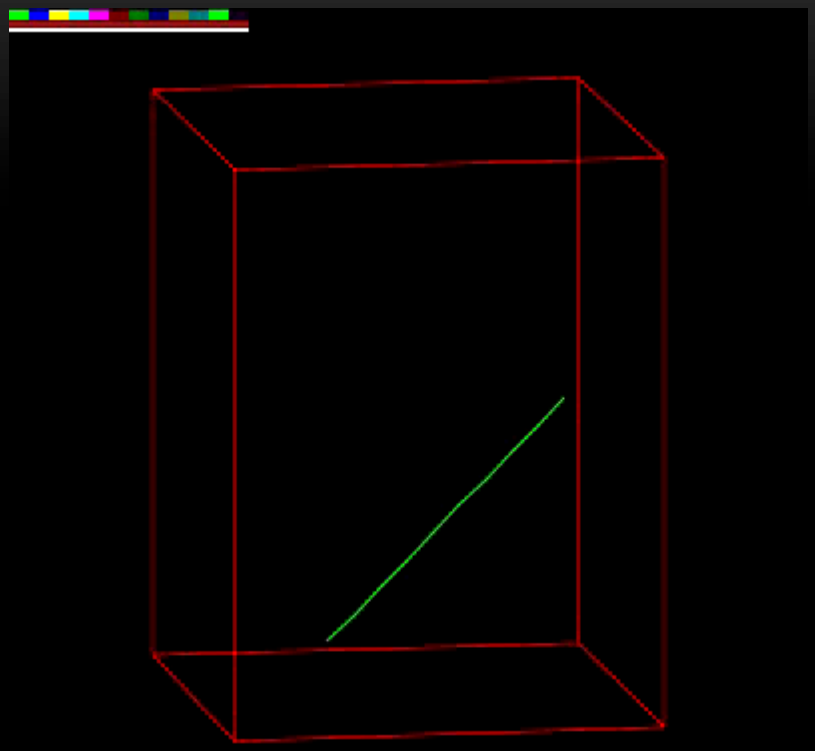
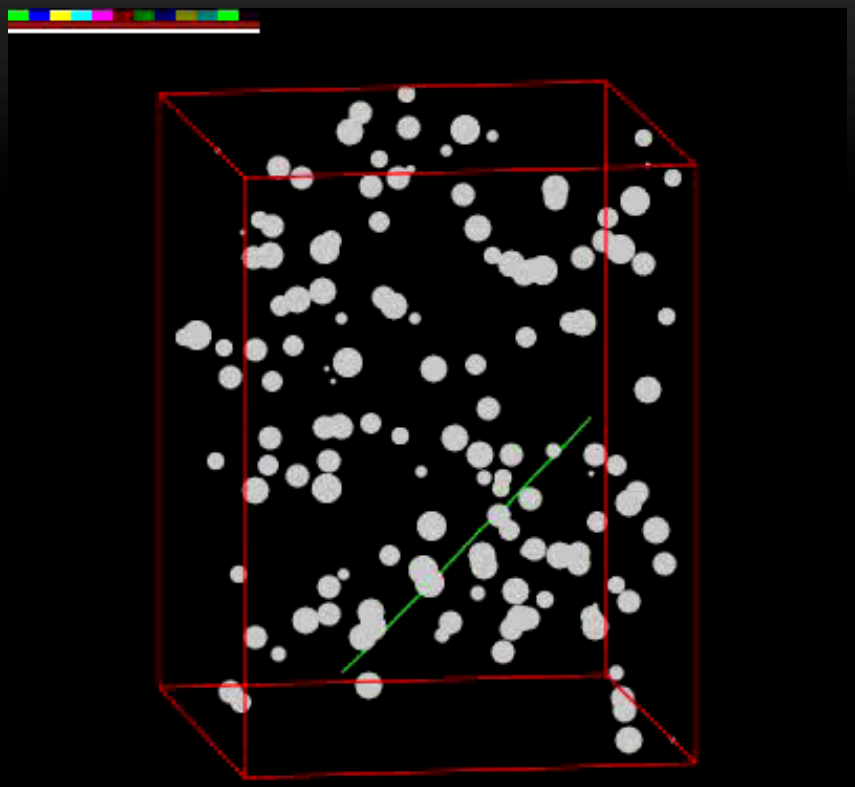
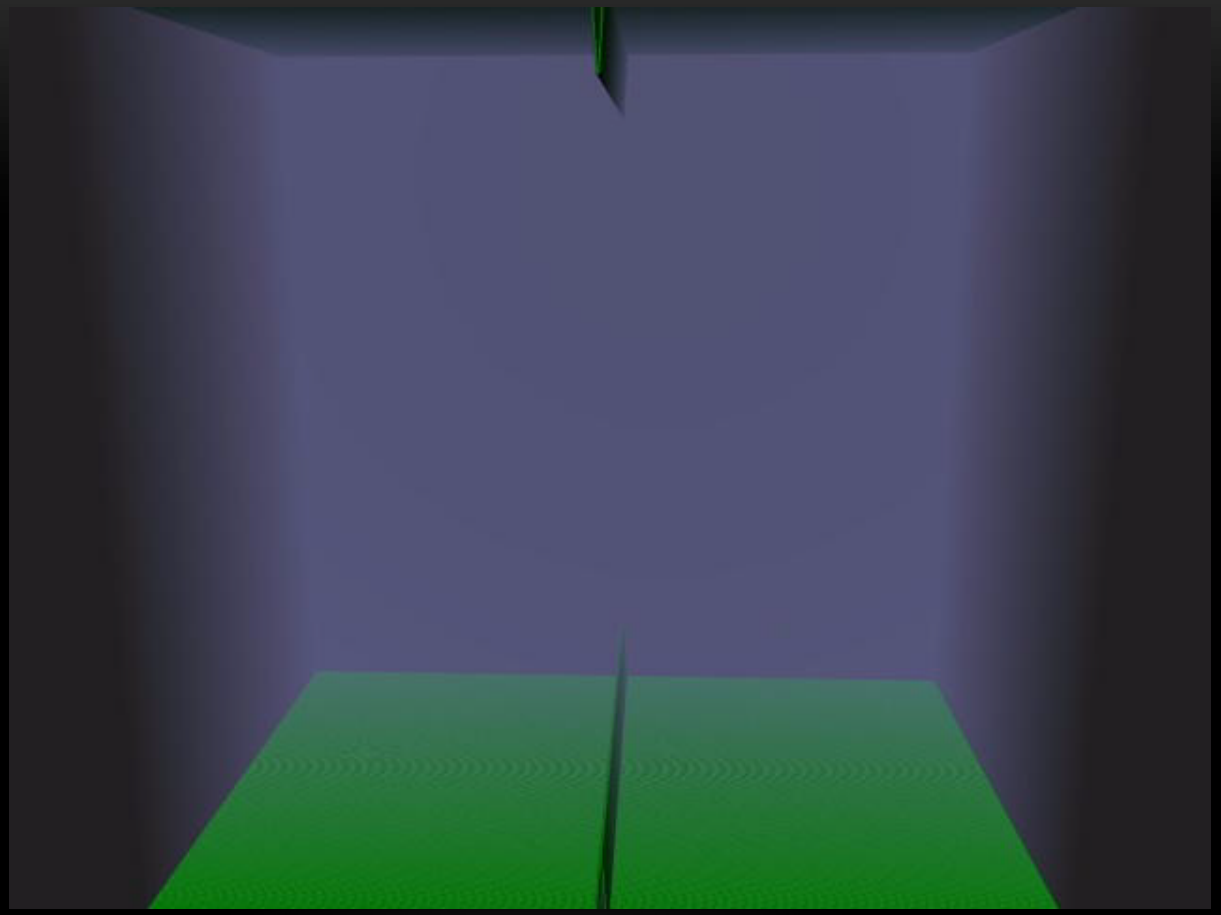




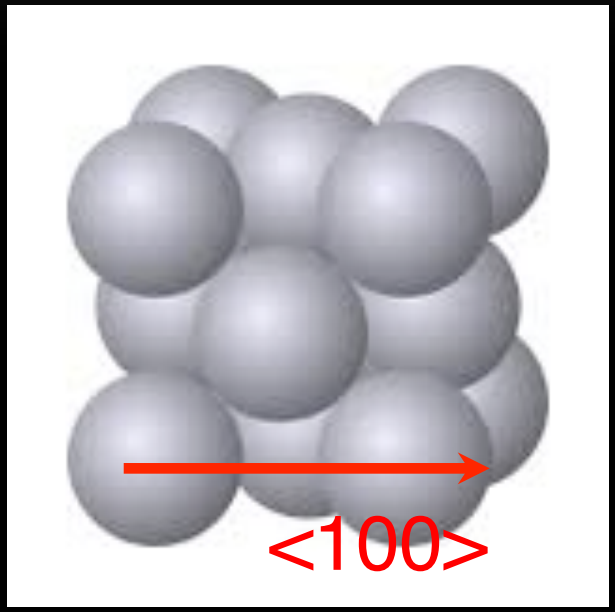
http://lem.onera.fr/DisGallery/source.html

MD SIMULATION OF DISLOCATIONS

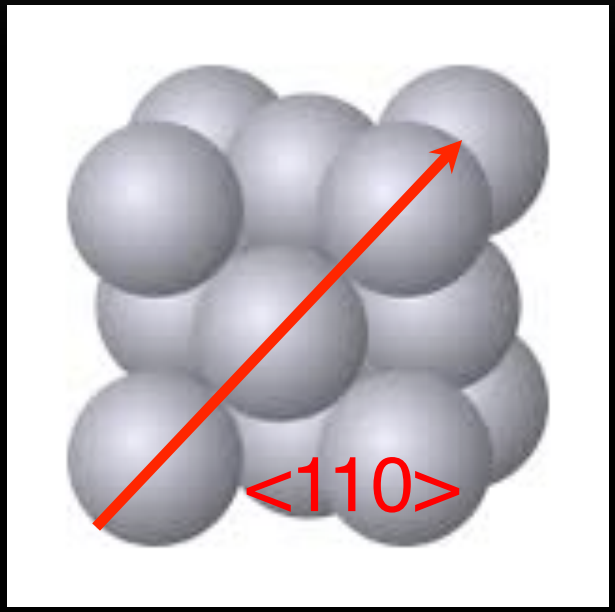


Farid Abraham of IBM Almaden Research, in collaboration with LLNL personnel Mark Duchaineau and Tomas Diaz De La Rubia.

DISLOCATIONS IN REAL CRYSTALS: FACE CENTERED CUBIC CRYSTALS



DISLOCATIONS IN REAL CRYSTALS: FACE CENTERED CUBIC CRYSTALS

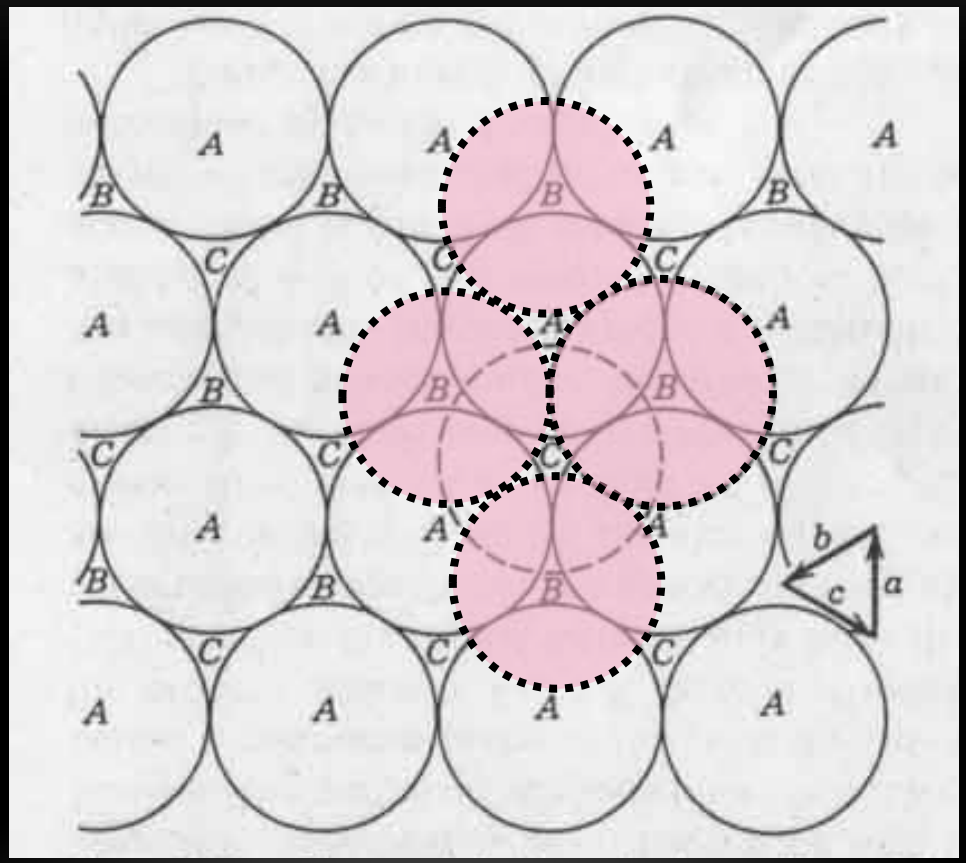


DISLOCATIONS IN REAL CRYSTALS: FACE CENTERED CUBIC CRYSTALS

{111} planes

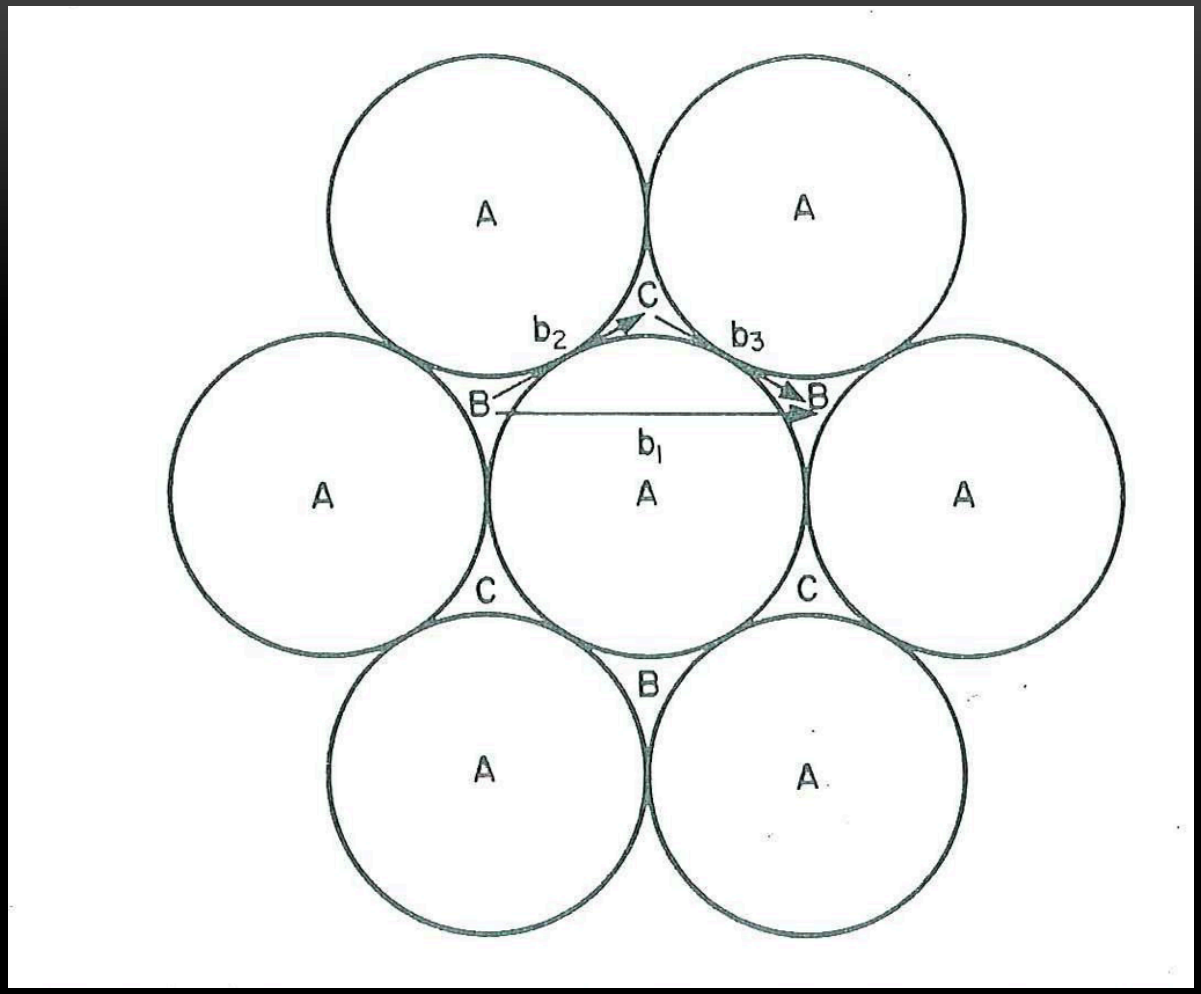
FCC: ABCABC

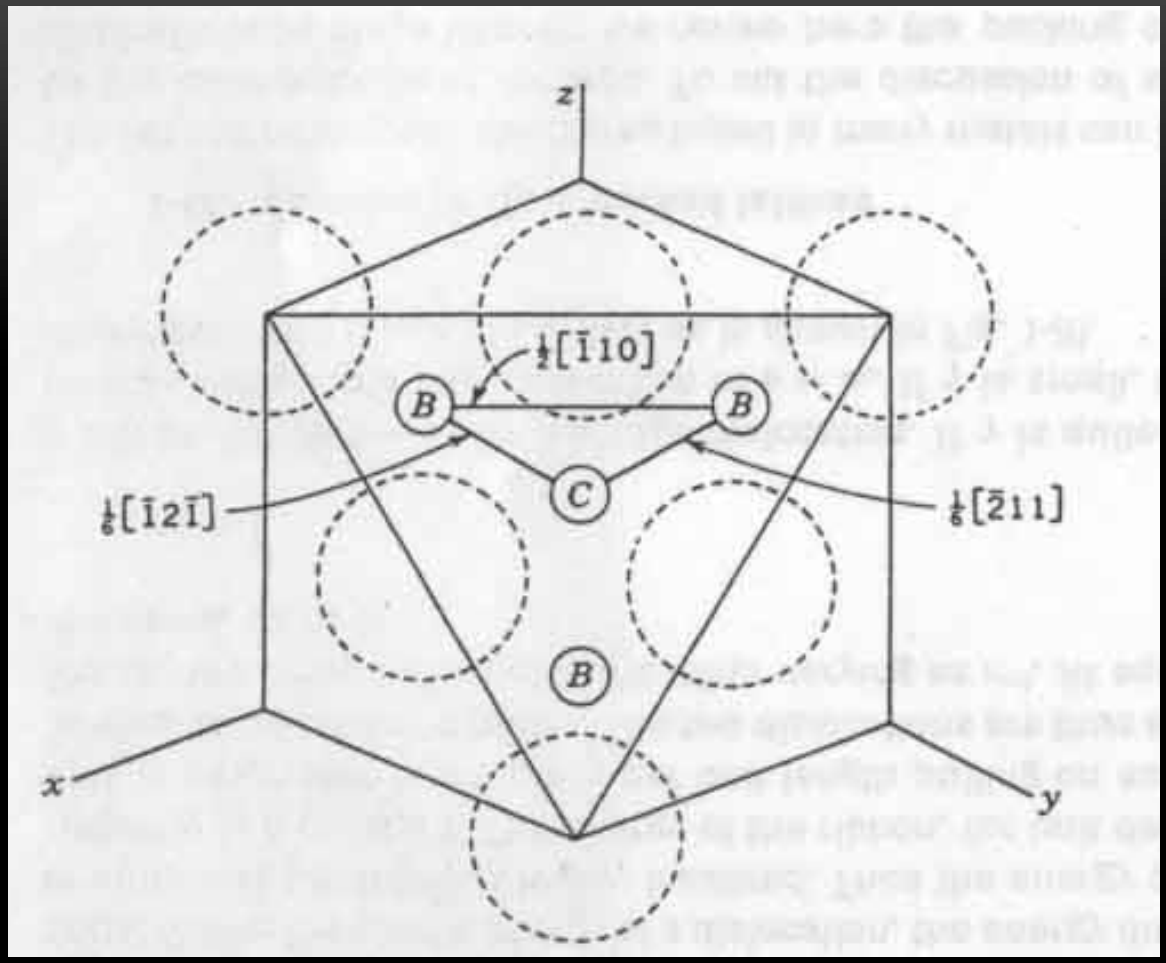
HCP: ABABAB



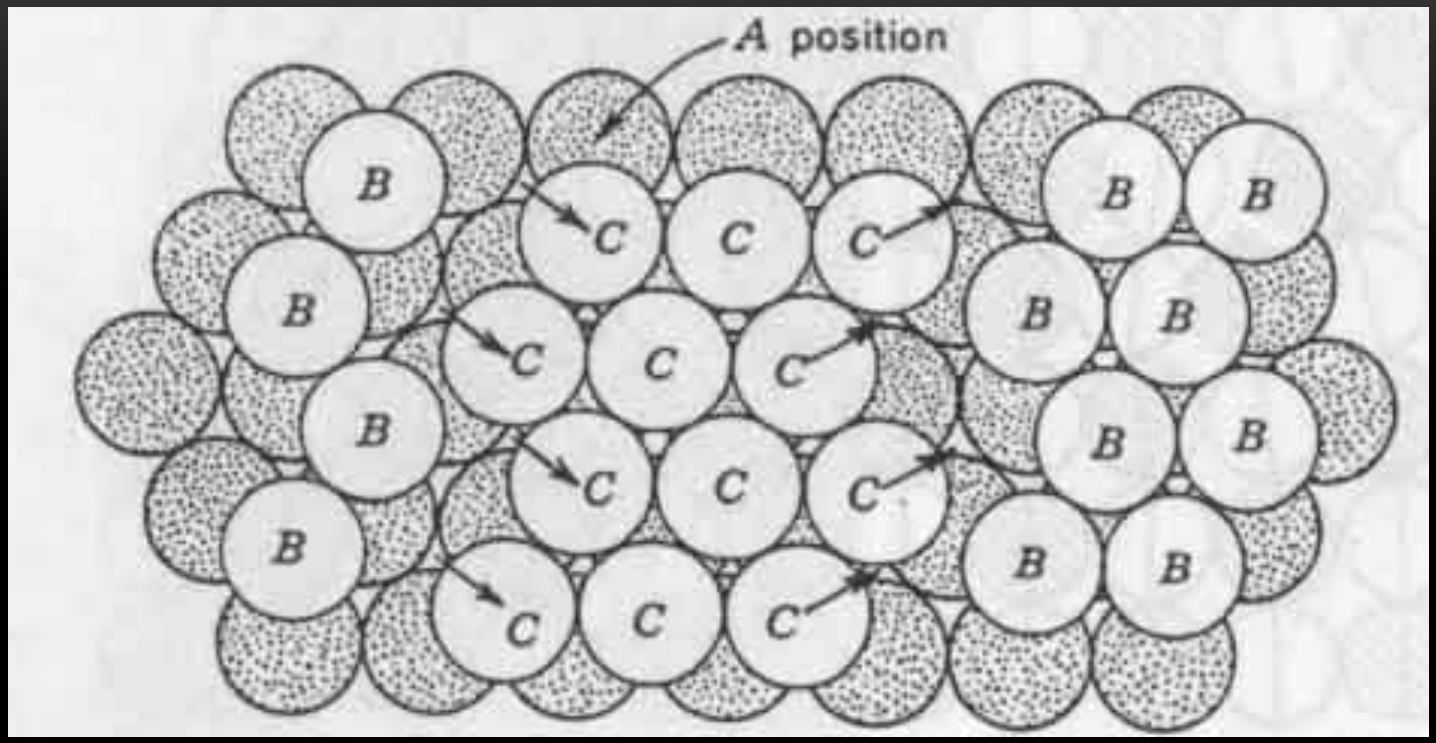
b_1 is a perfect dislocation

b_2, b_3 are Shockley partial dislocations



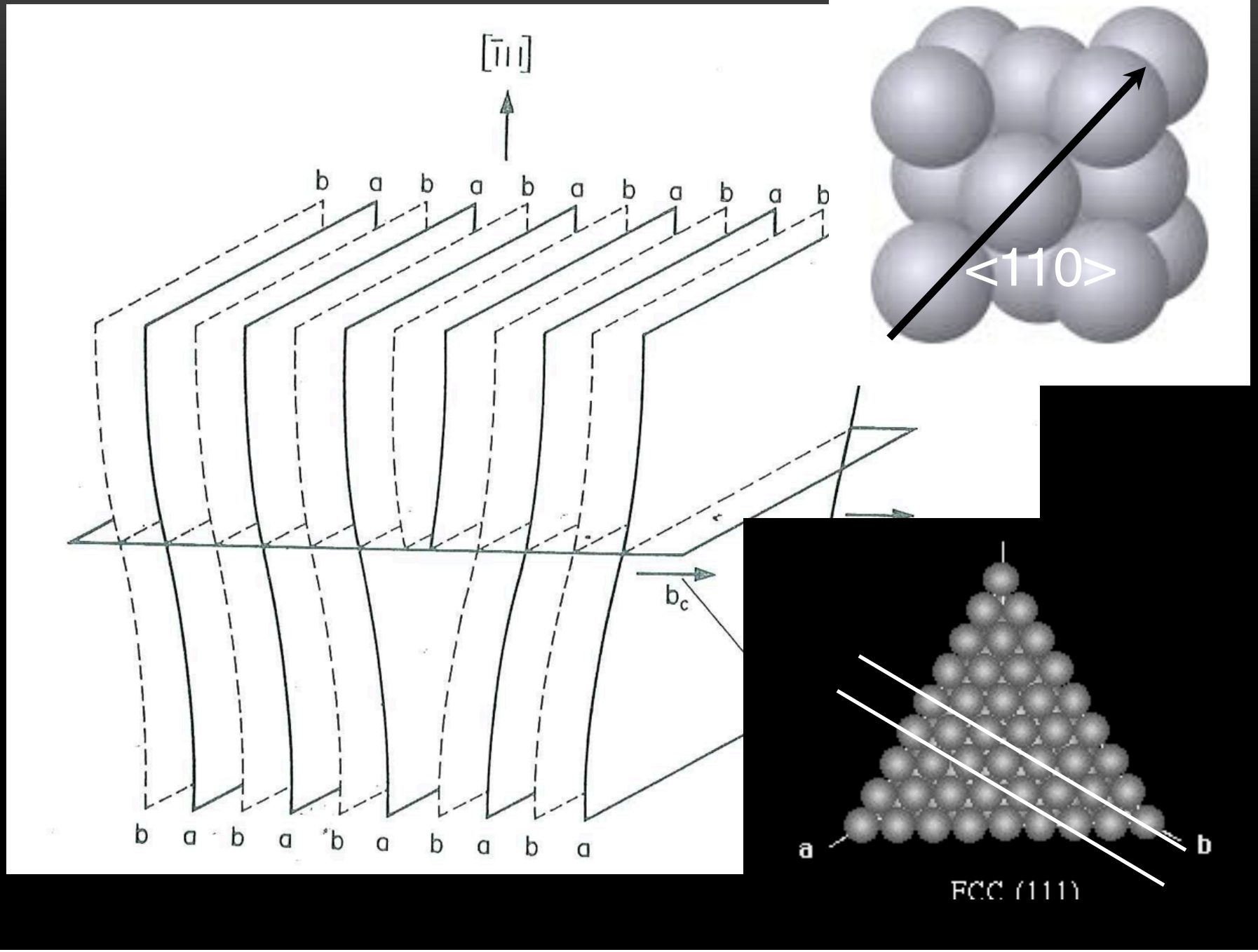


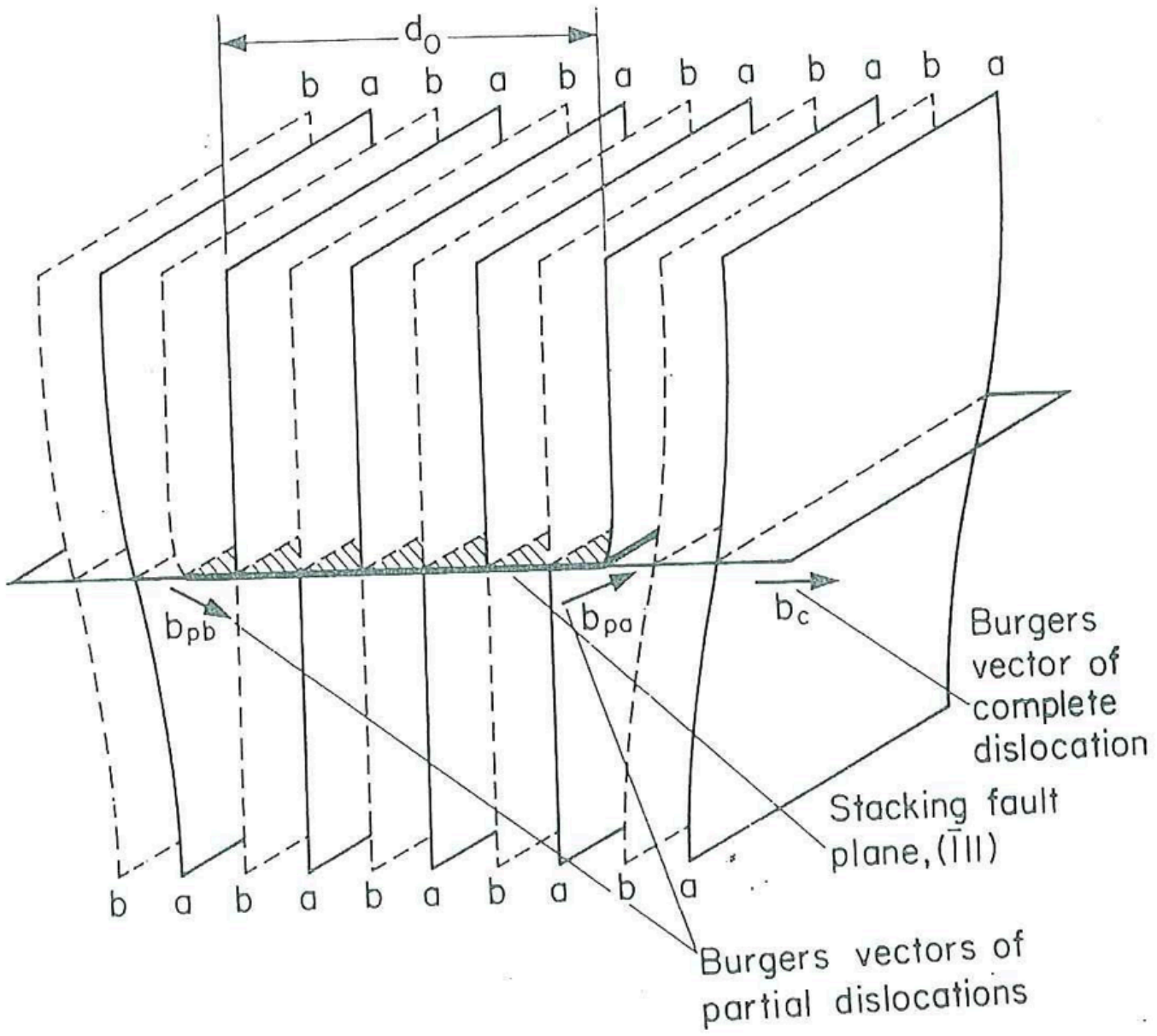
$$\frac{1}{2}[\overline{1}10] \rightarrow \frac{1}{6}[\overline{1}2\overline{1}] + \frac{1}{6}[\overline{2}11]$$

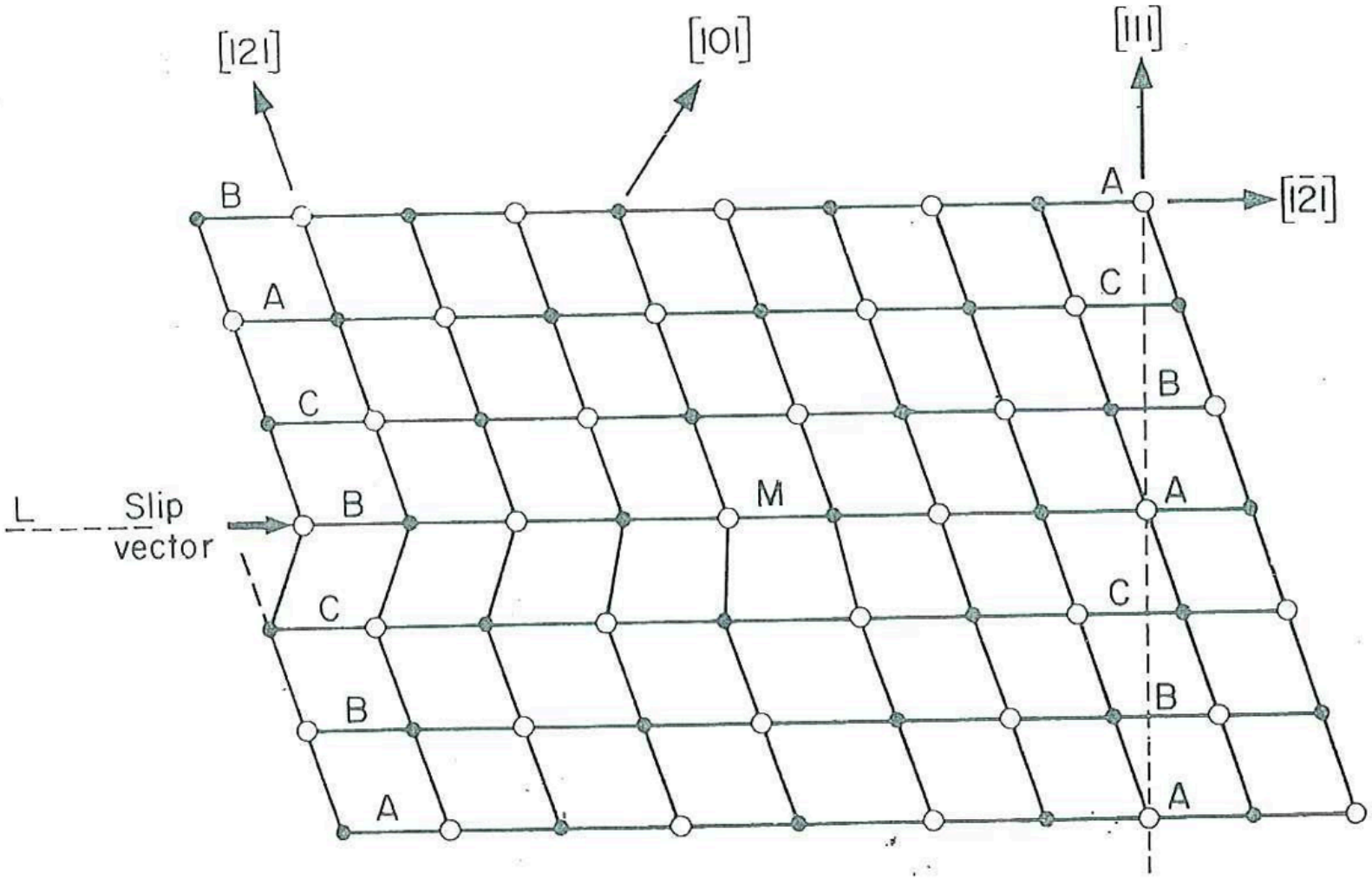


Stacking fault!

Energy of a stacking fault is small: correct nearest neighbors, incorrect second nearest neighbors


[$\bar{1}$11]
b a b a b a b a b a b a b
b a b a b a b a b a
b_c
<110>
a
b
FCC (111)


d_0
b a b a b a b a b a b a b a
b_{pb}
b_{po}
b_c
Burgers vector of complete dislocation
Stacking fault plane, $(\bar{1}11)$
b a b a b a b a b a
Burgers vectors of partial dislocations


[12̄1]
[101]
[111]
[1̄21]
B
A
C
B
A
C
B
M
A
C
B
A
L
Slip
vector

Force between two partial dislocations is, approximately,

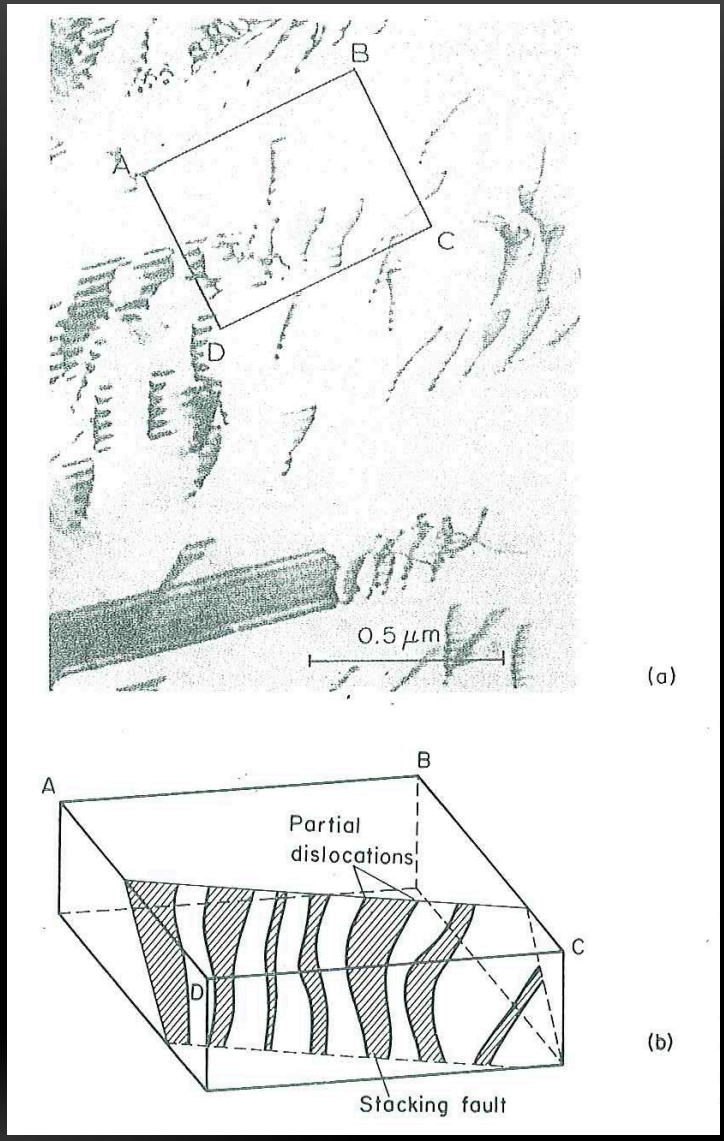
$$F' = \frac{\mu \mathbf{b}_1 \cdot \mathbf{b}_2}{2\pi d}$$

The stacking fault energy:

$$\gamma_{st} = \frac{\text{energy}}{\text{area}} = \frac{\text{force}}{\text{length}}$$

Equating the two gives the equilibrium stacking fault width

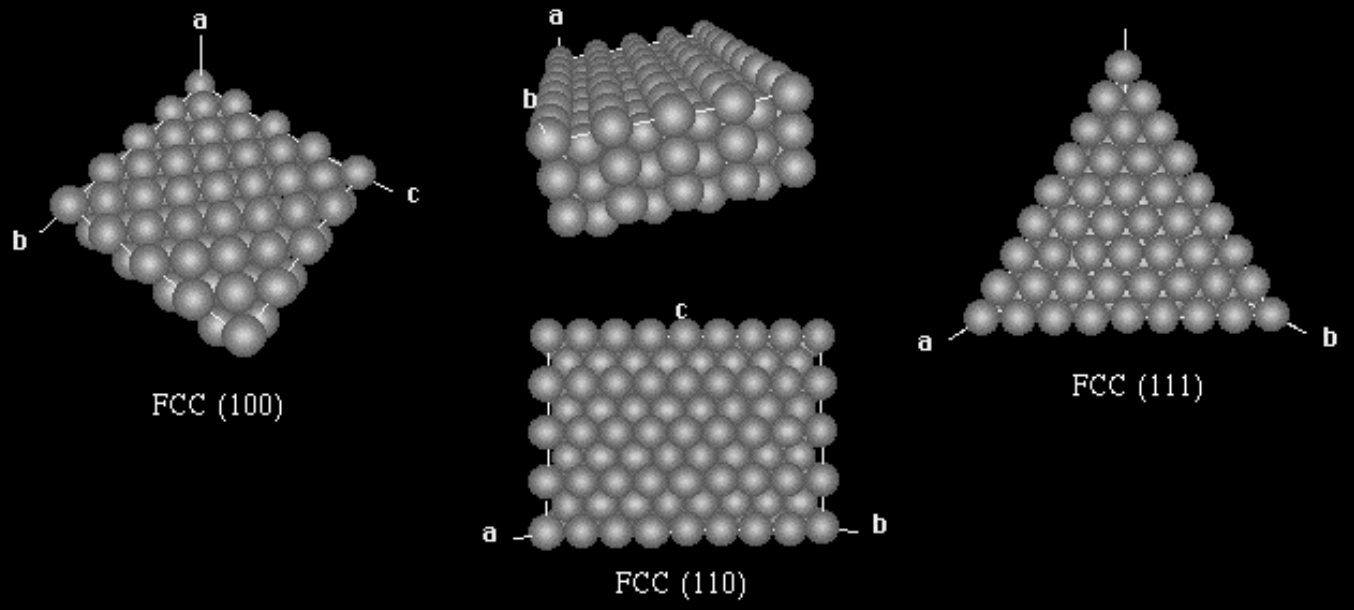
$$d = \frac{\mu b^2}{4\pi \gamma_{sf}}$$



Which for copper yields d = 5a for γ_{sf} of 40mJ/m^2

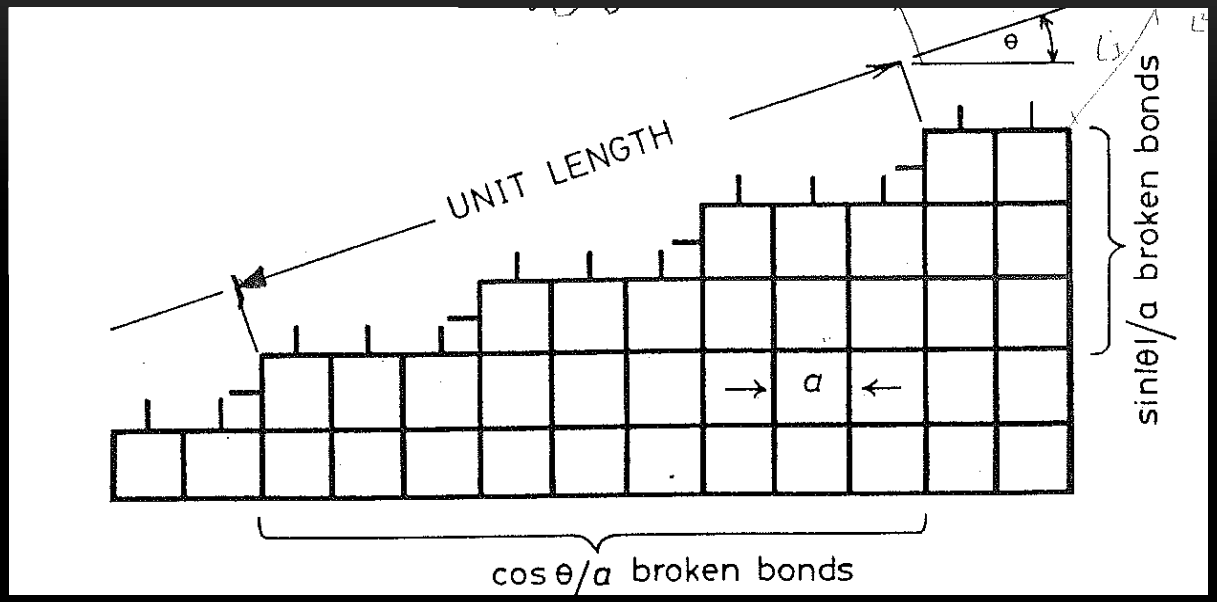
INTERFACES IN CRYSTALS

- Surface energy is a result of missing bonds at the surface



- Surface energy scales with the bond strength and the number of missing bonds

INTERFACIAL ANISOTROPY



$$E_{sv} = \frac{e_b}{2a^2} \left(|\cos(\theta)| + |\sin(\theta)| \right)$$

INTERFACIAL ANISOTROPY

Equilibrium shape is given by a minimum in:

$$\int_s \gamma(\mathbf{n}) ds$$

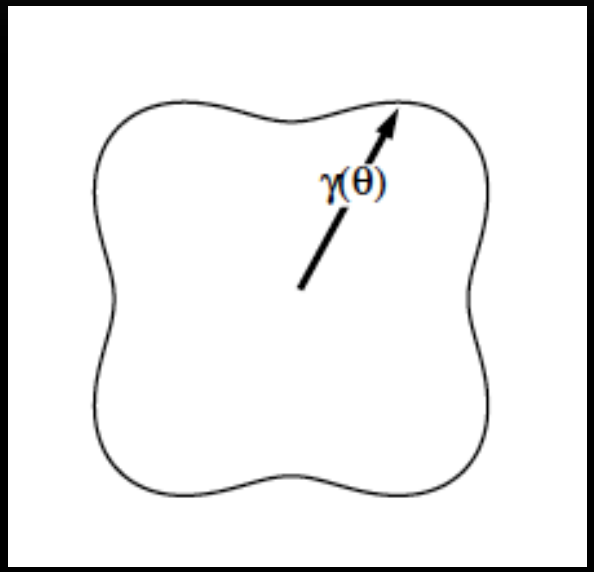
subject to the constraint:

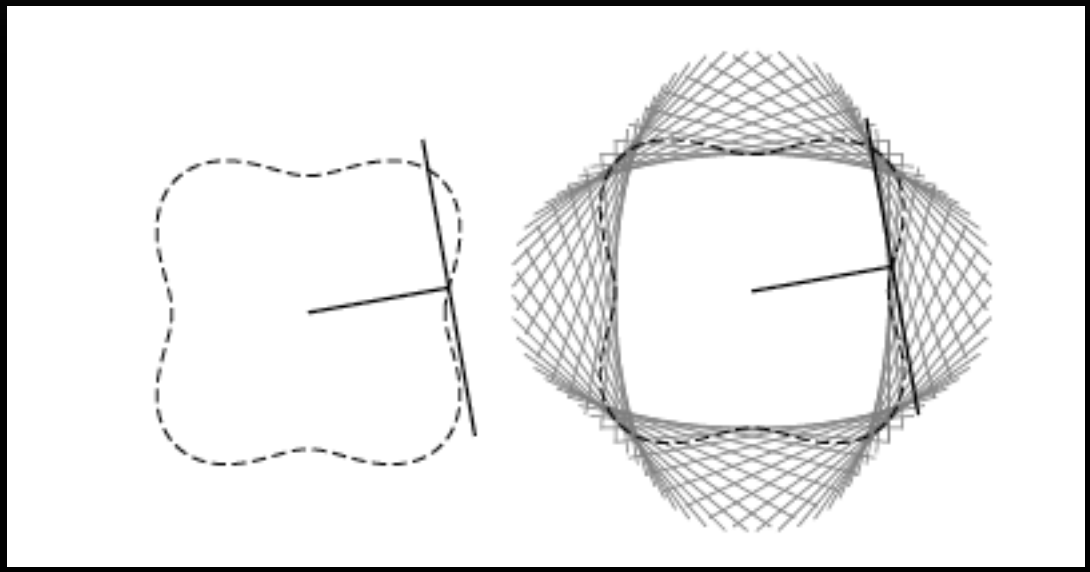
$$V = \text{constant}$$

Answer: Wulff construction

http://www.wired-artist-jewelry.com/STONES/qtzspec.jpg

WULFF CONSTRUCTION



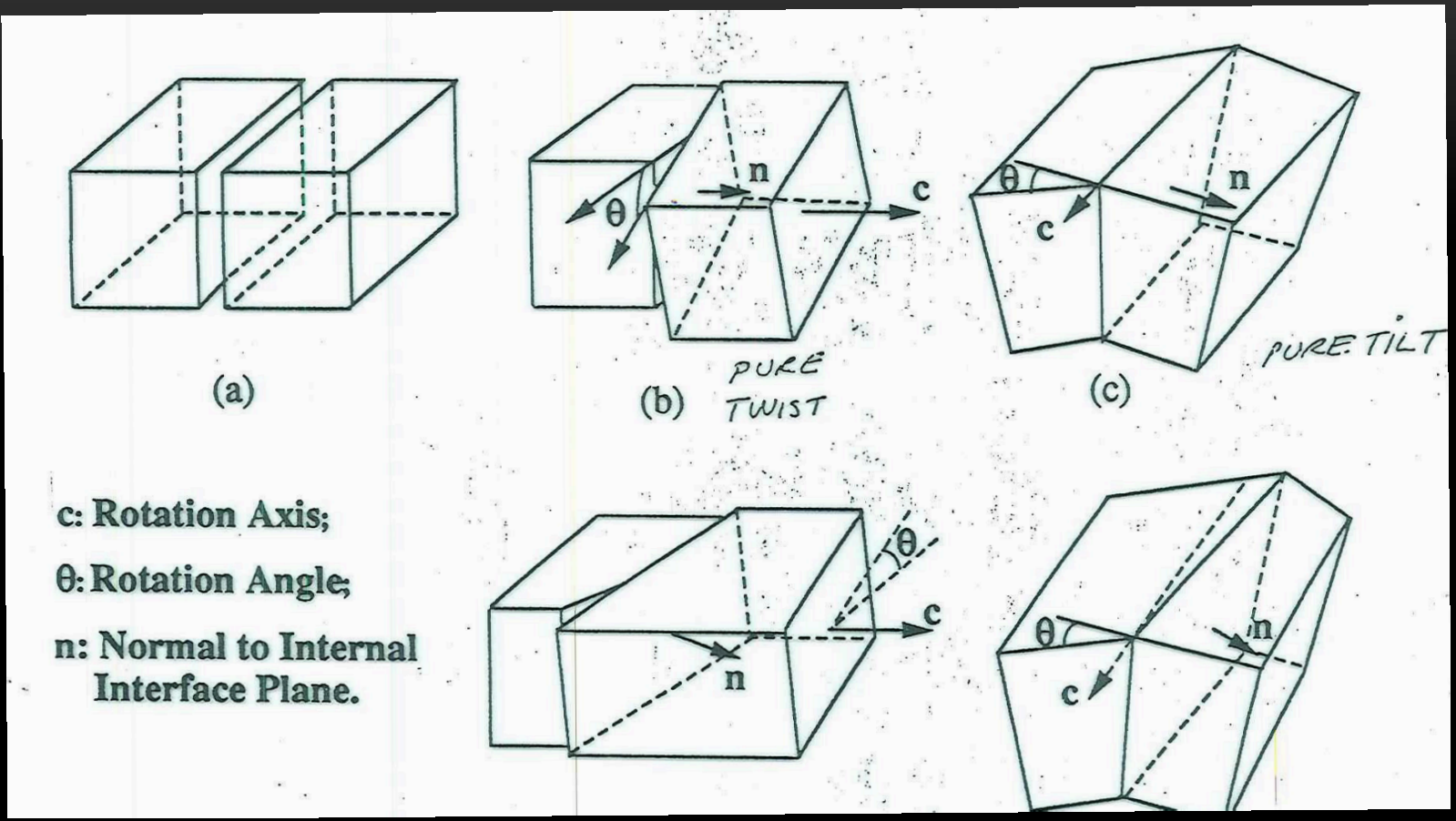


(W.C. Carter, lecture notes)

GRAIN BOUNDARIES

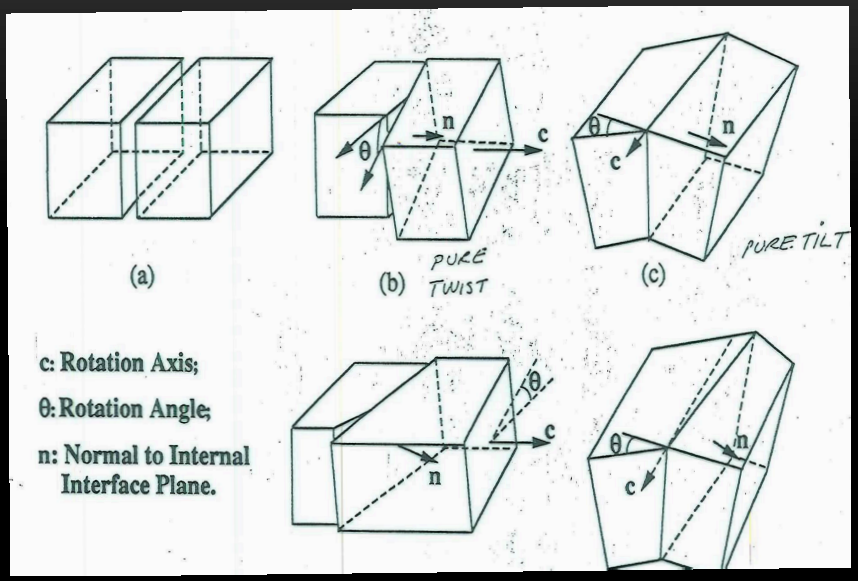
- A. Sutton and R. Balluffi (1996), *Interfaces in Crystalline Materials*, Oxford.
- Adam J. Schwartz and Mukul Kumar, *Electron Backscatter Diffraction in Materials Science*, 2nd Ed., Springer, 2009.
- Morawiec, A. (2003), *Orientations and Rotations*, Berlin: Springer.
- V. Randle & O. Engler (2009). *Texture Analysis: Macrotexture, Microtexture & Orientation Mapping*. 2nd Ed. Amsterdam, Holland, CRC Press.
- Gottstein and Shvindlerman, *Grain Boundary Migration in Metals: Thermodynamics, Kinetics, Applications*, CRC Press (2009).

GRAIN BOUNDARIES: DEGREES OF FREEDOM



Pure twist C and n parallel. Pure tilt C and n perpendicular

GRAIN BOUNDARIES: DEGREES OF FREEDOM



C is a unit vector, (c_1, c_2, c_3) , 2 degrees of freedom

n is a unit vector, (n_1, n_2, n_3), 2 degrees of freedom

θ, 1 degree of freedom

Thus there are 5 macroscopic degrees of freedom

LOW ANGLE GRAIN BOUNDARIES: SYMMETRIC TILT

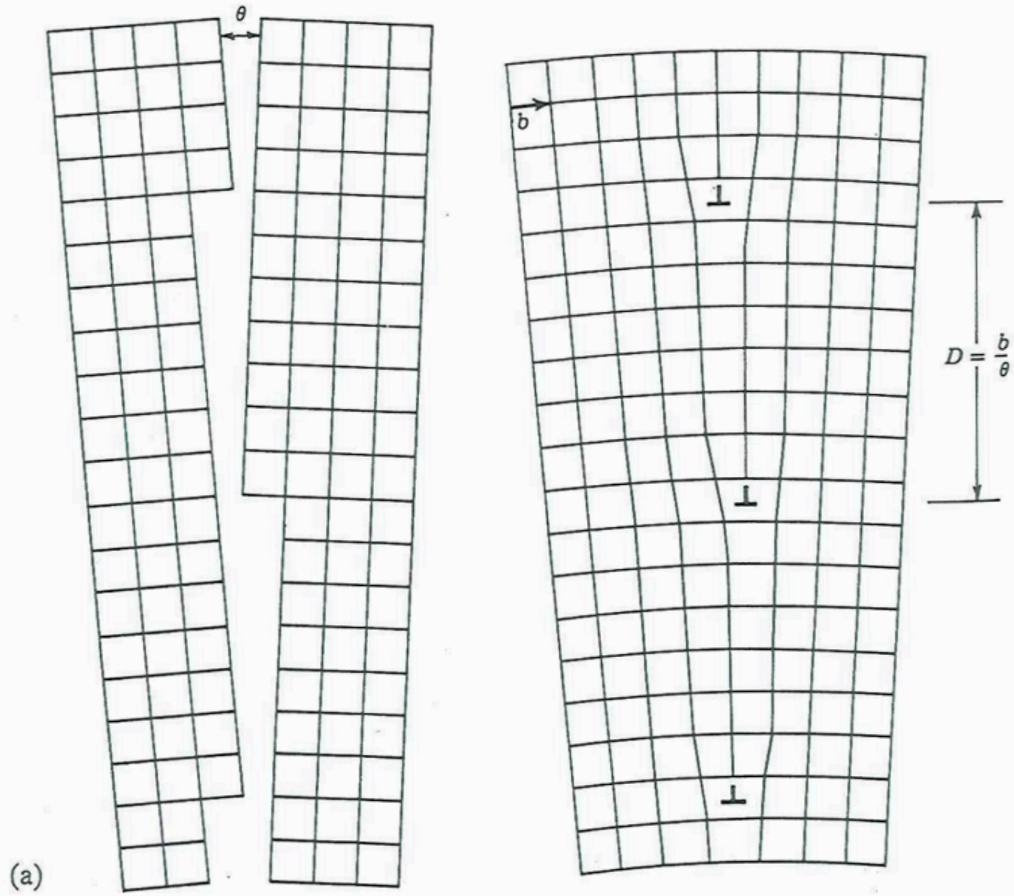
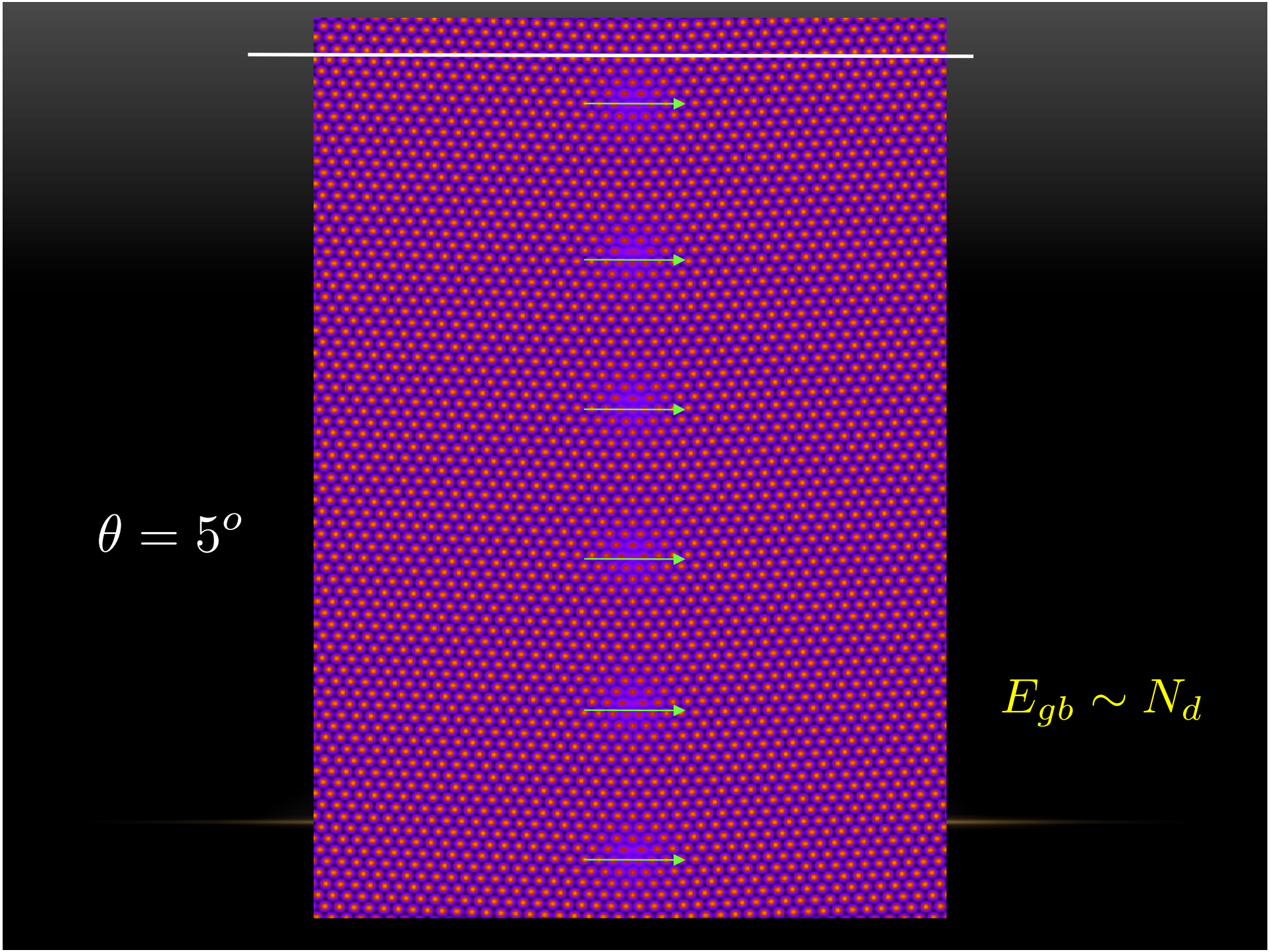
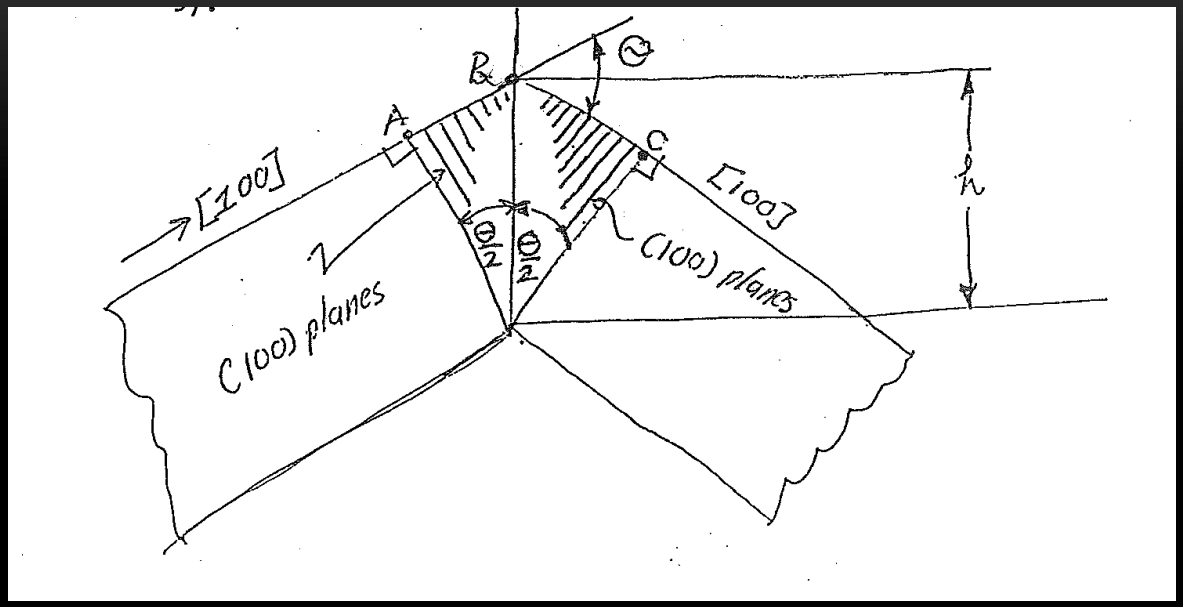


Fig. 3.7 (a) Low-angle tilt boundary, (b) low-angle twist boundary: ○ atoms in crystal below boundary, ● atoms in crystal above boundary. (After W.T. Read Jr., *Dislocations in Crystals*, McGraw-Hill, New York, 1953.)


$\theta = 5^o$
$E_{gb} \sim N_d$

NUMBER OF DISLOCATIONS IN A TILT BOUNDARY



$$BC = h\sin(\theta/2)$$

$$n_p b = 2h\sin(\theta/2)$$

$$D = \frac{h}{n_P} = \frac{b}{2\sin(\theta/2)}$$

NUMBER OF DISLOCATIONS IN A TILT BOUNDARY

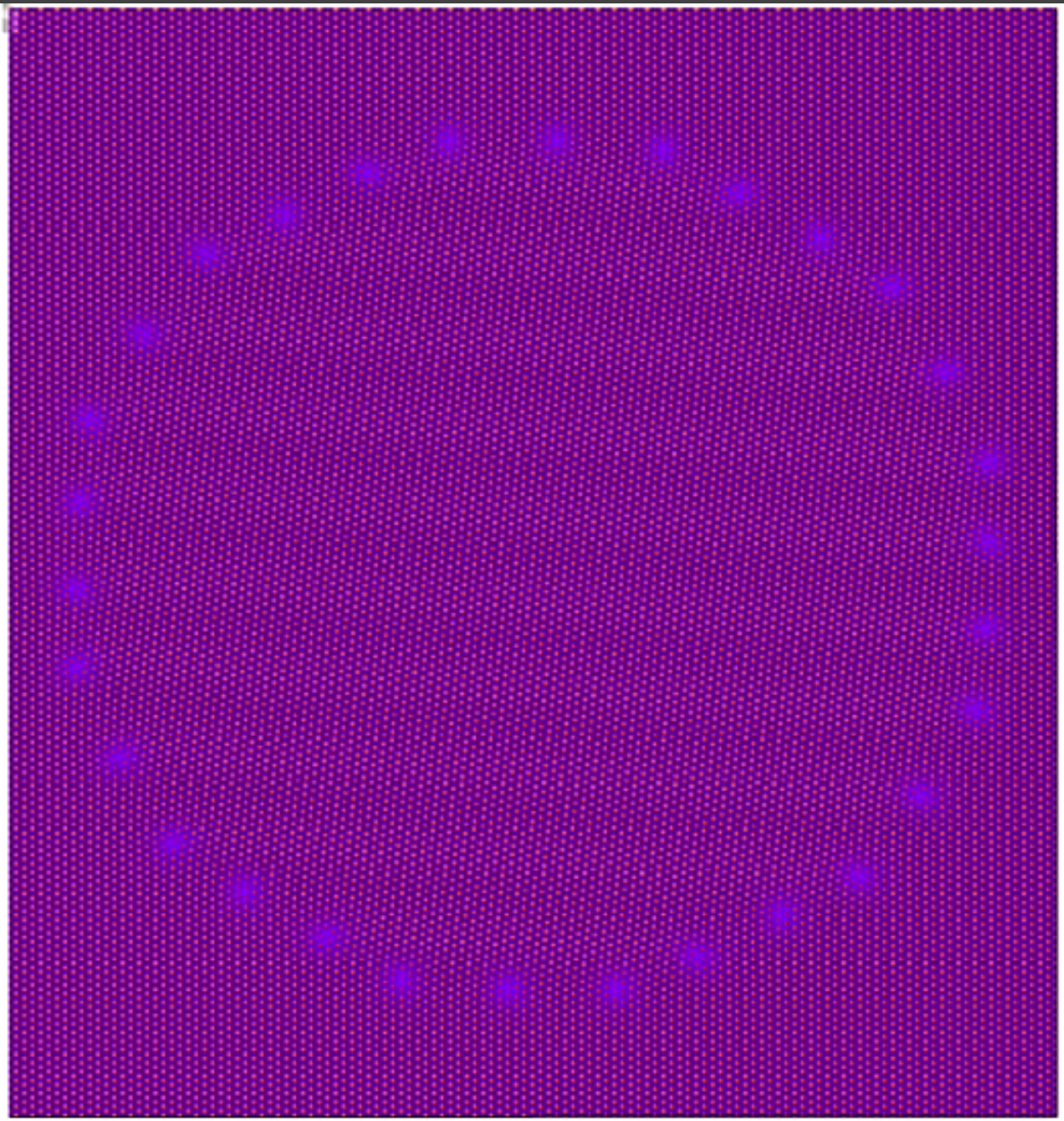
- For small θ,

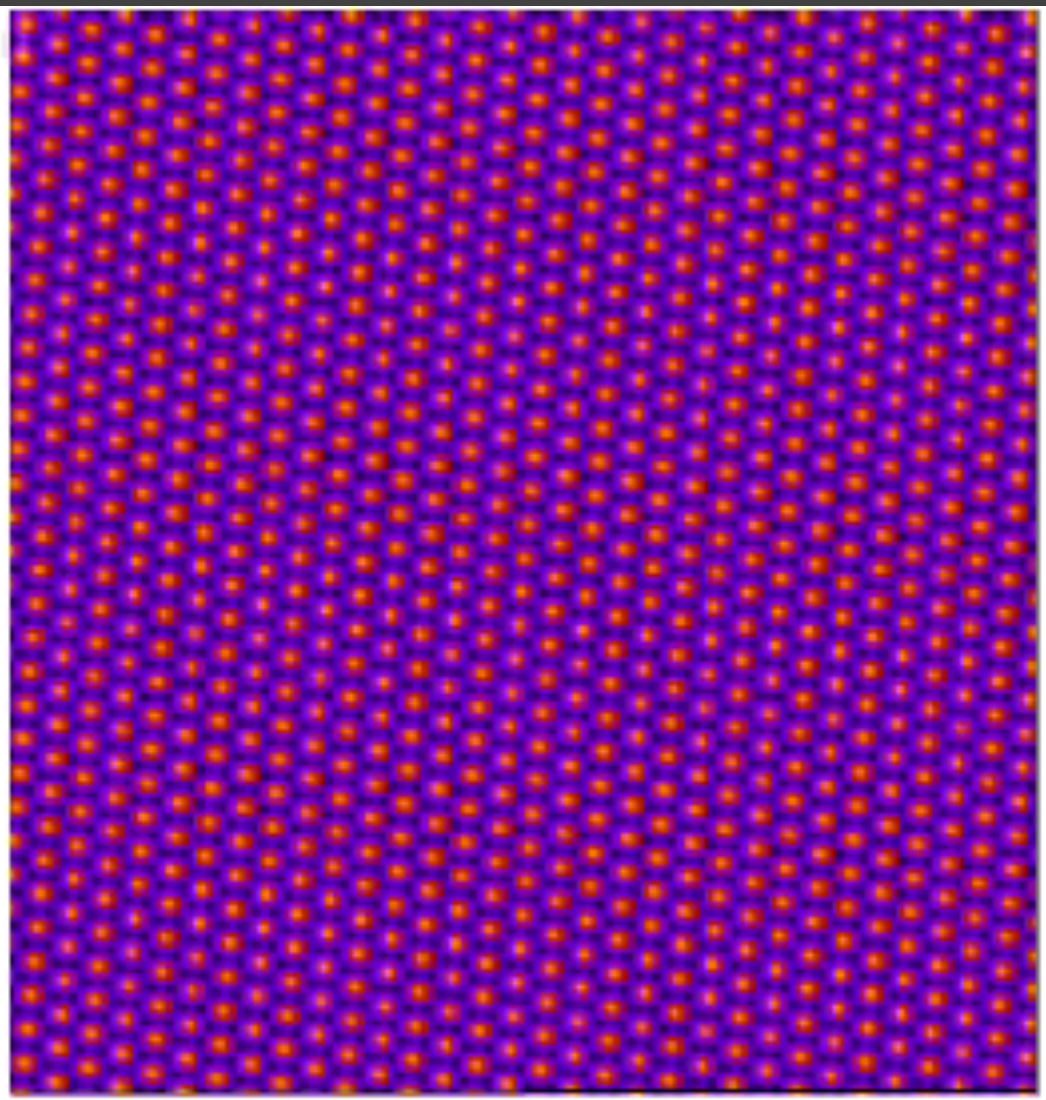
$$D = \frac{b}{\theta} \qquad n_p = \frac{h}{b}\theta$$

- The energy should also be linear in θ for small θ
- Read Shockley:

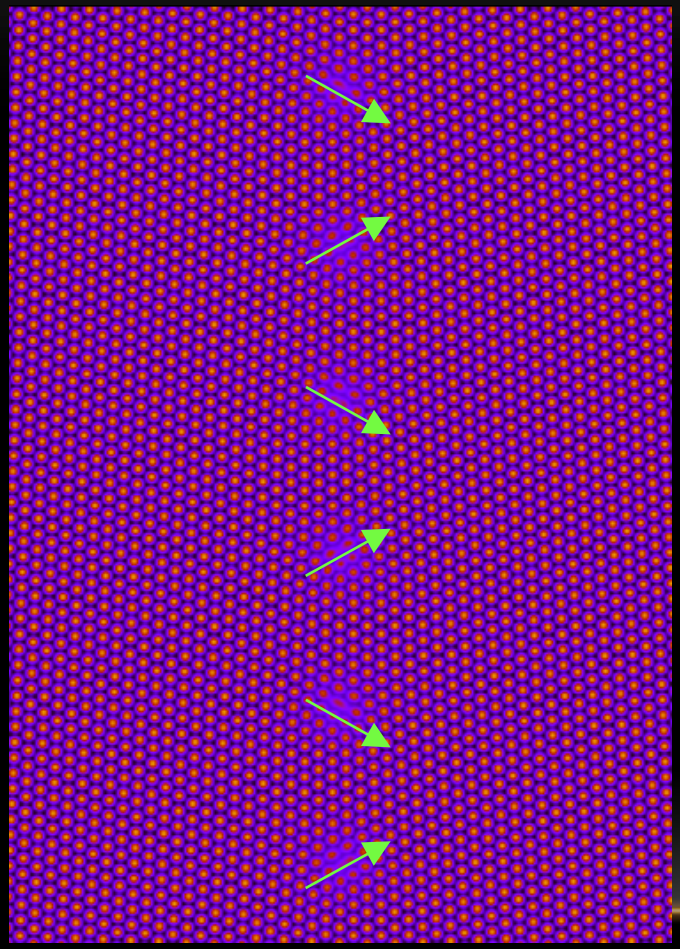
$$\gamma_{GB} = \frac{bE}{8\pi}\theta\left(B - \ln\theta\right)$$

- For large θ, b is on the order of D, and it is not possible to define a dislocation: “high angle” grain boundaries


t=0010000


t=0010000

WHAT HAPPENS IF THE NORMAL TO THE PLANE IS CHANGED?

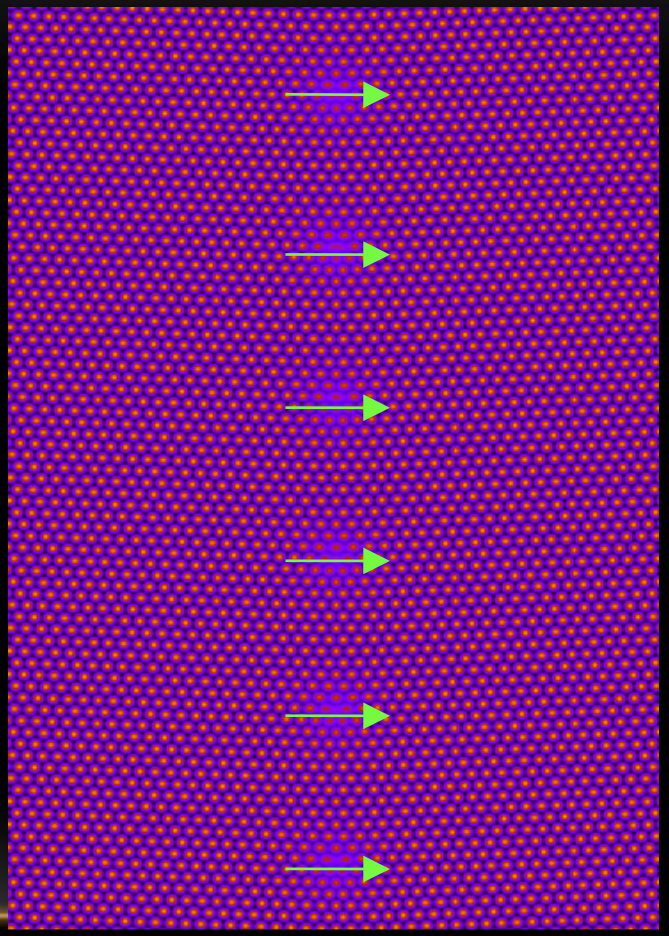


$\phi = 0^o$

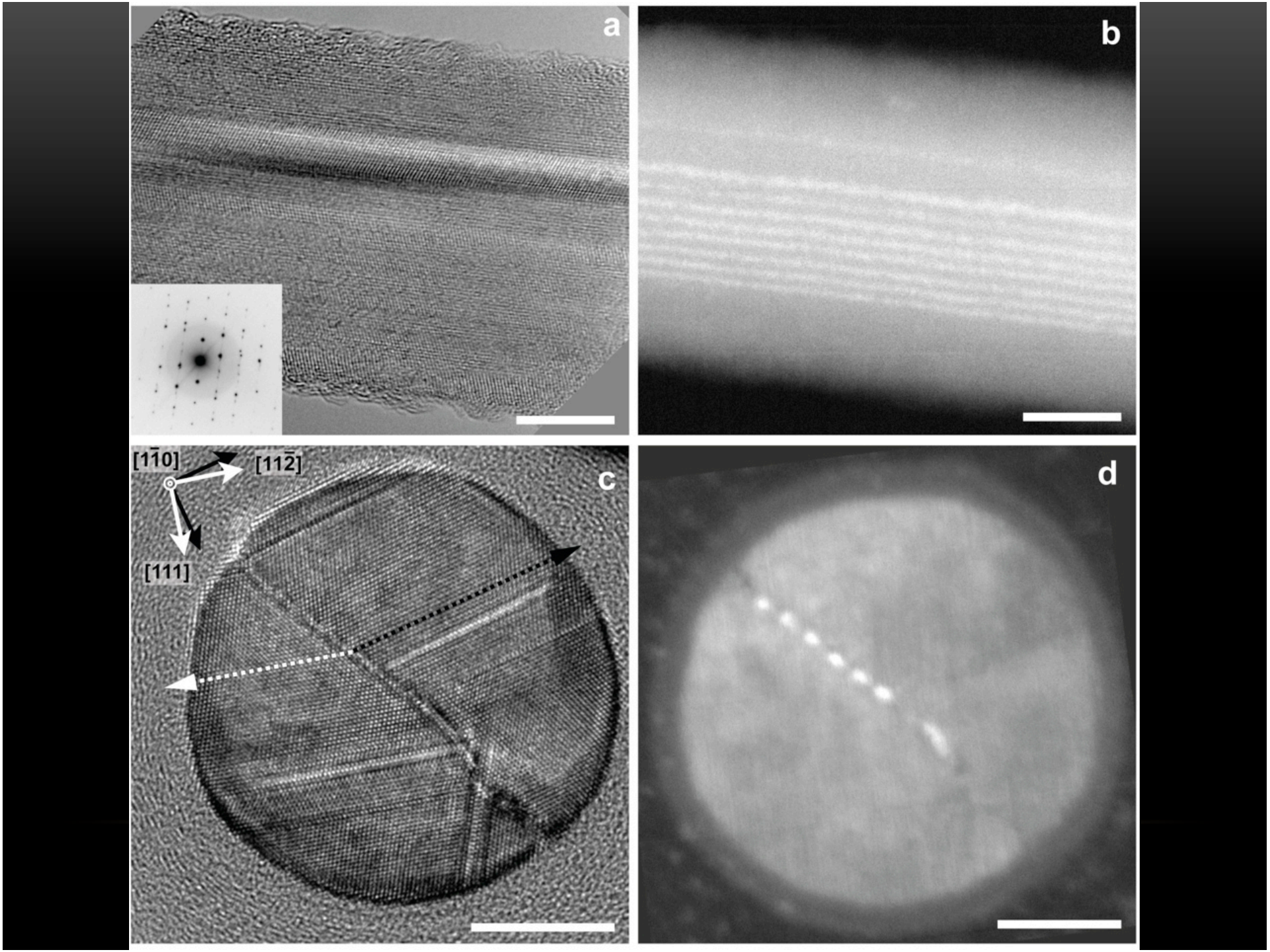
$\theta = 5^o$

Frank Formula

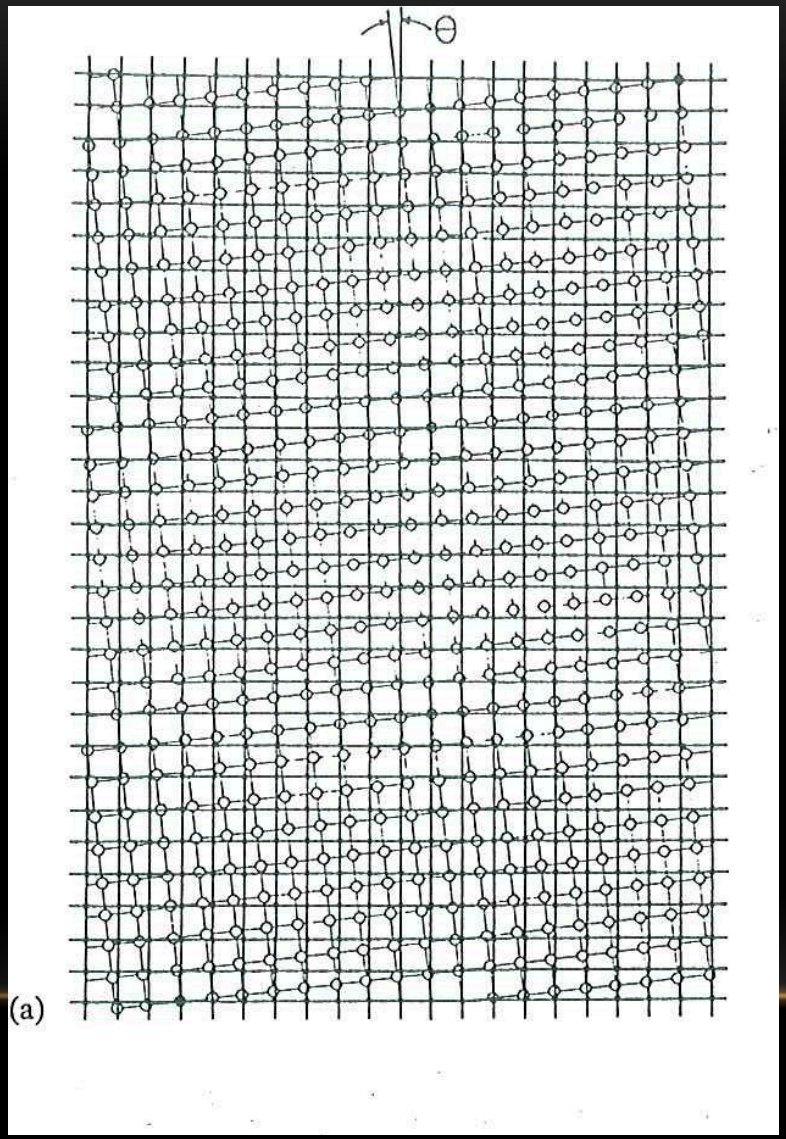
$$\mathbf{n}_b = (\mathbf{r} \times l)\,\theta$$



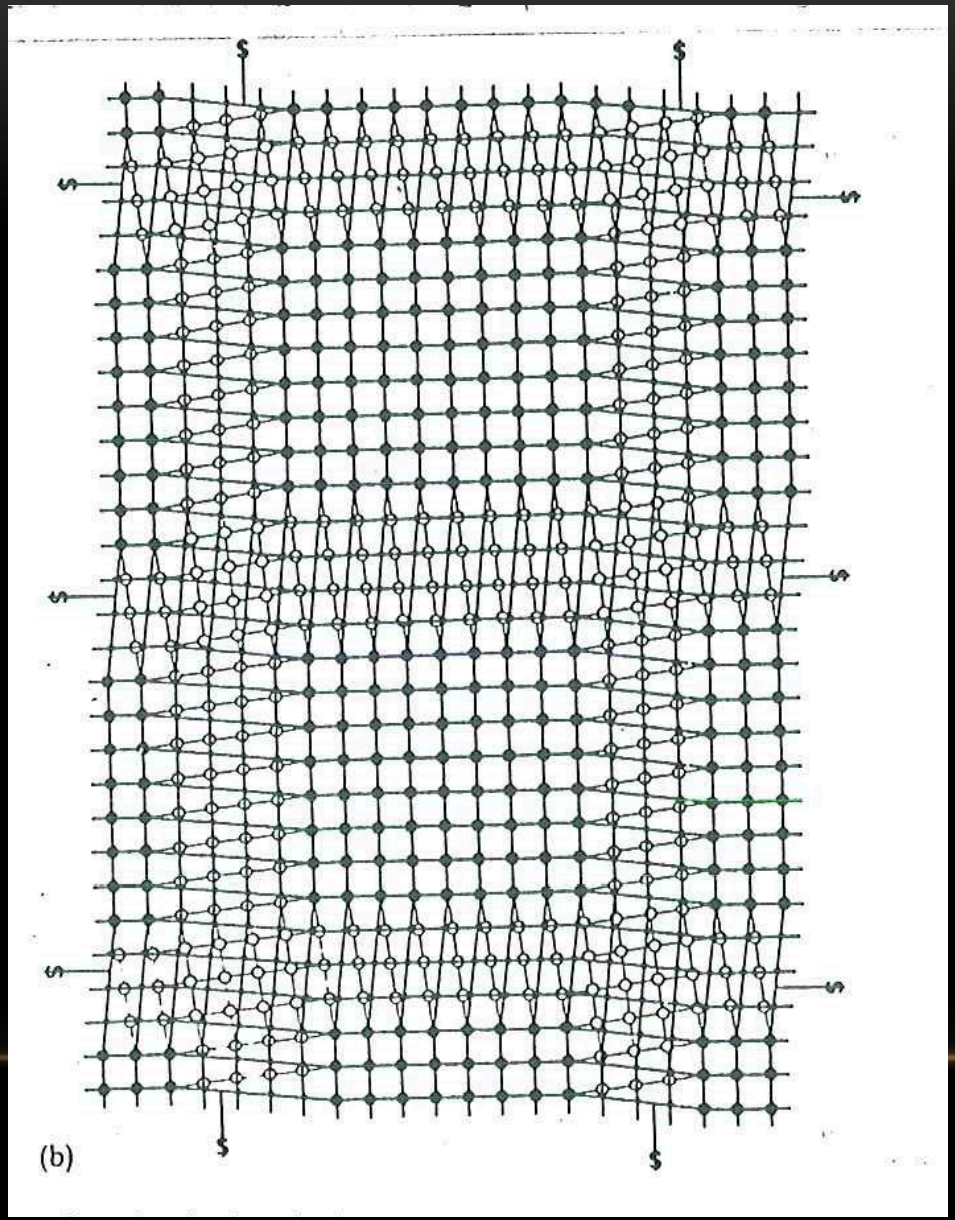
$\phi = 30^o$


a
b
c
d
[1$\bar{1}$0]
[11$\bar{2}$]
[111]

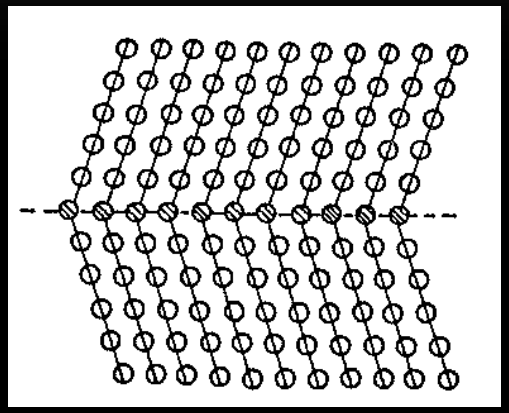
SIMPLE TWIST BOUNDARIES

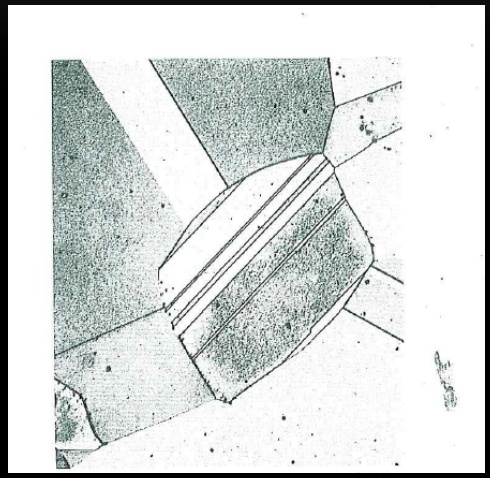


SIMPLE TWIST BOUNDARIES

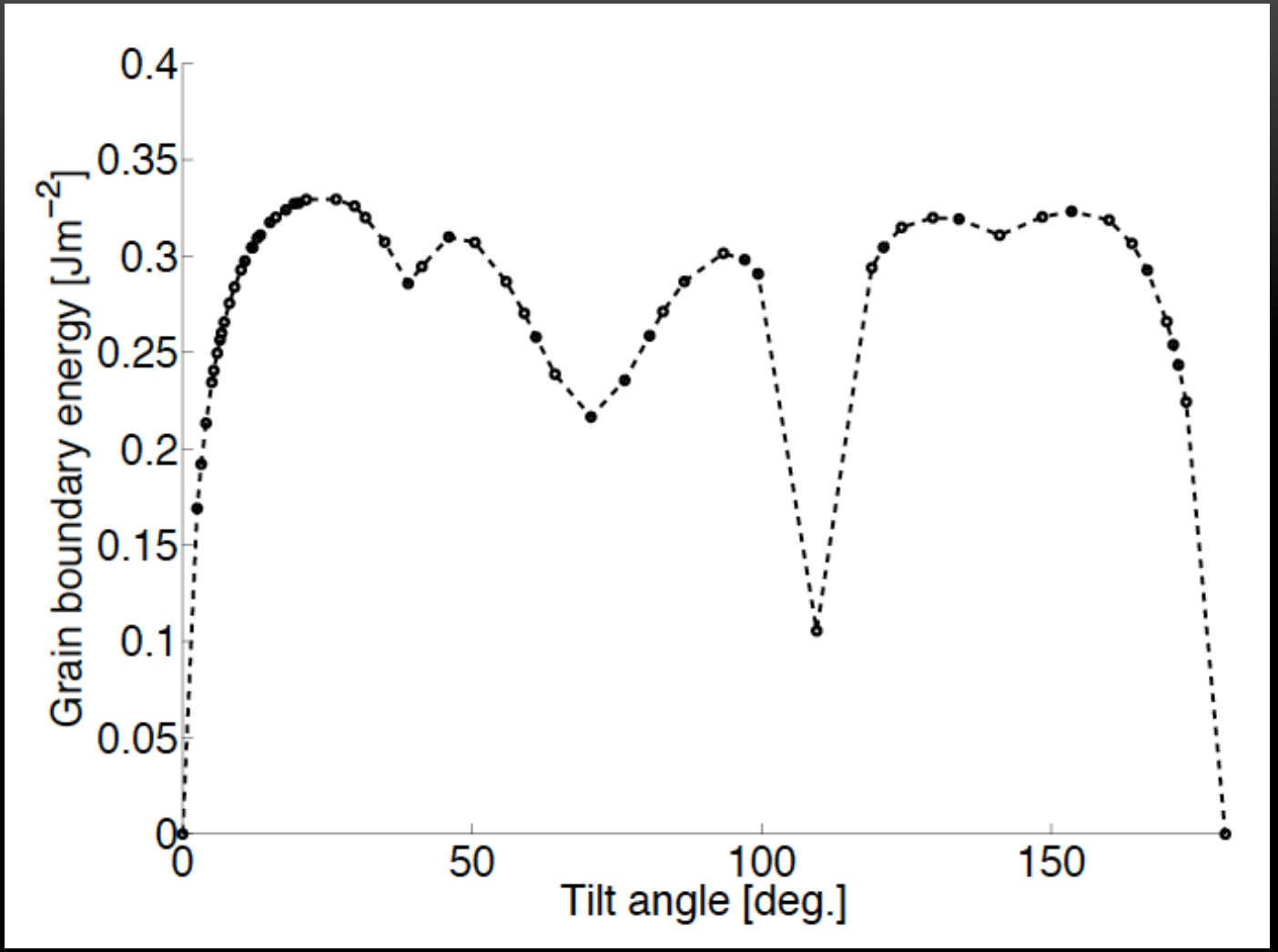


SPECIAL HIGH ANGLE GRAIN BOUNDARIES: TWINS



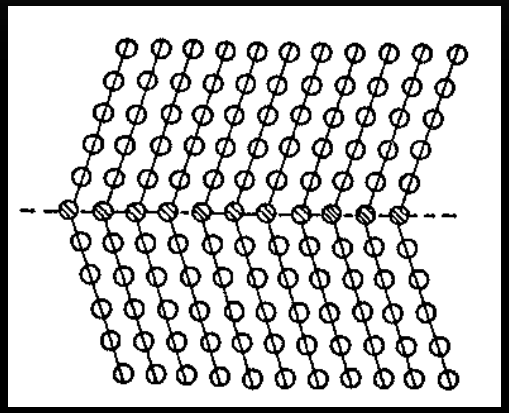


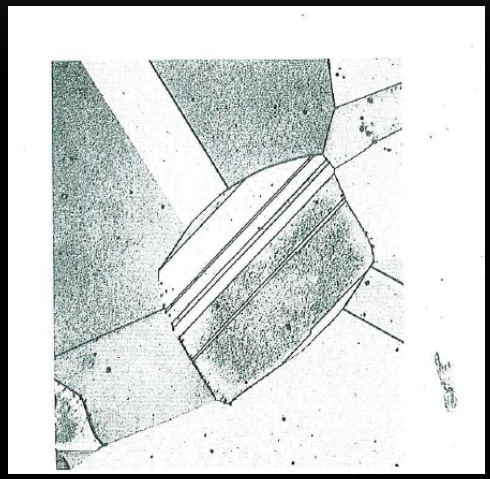
These are very low energy boundaries, no dislocations and a very regular arrangement of atoms



Grain boundary energy in iron

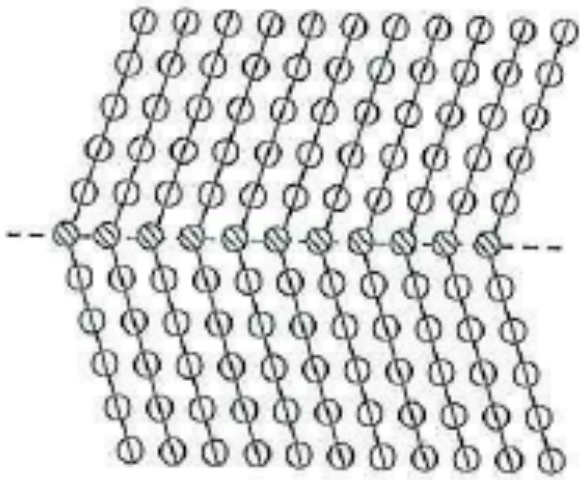
SPECIAL HIGH ANGLE GRAIN BOUNDARIES: TWINS



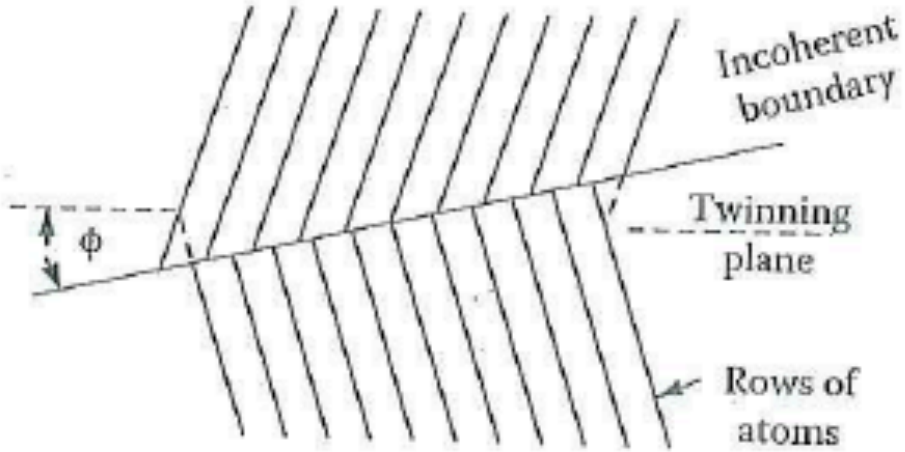


These are very low energy boundaries, no dislocations and a very regular arrangement of atoms

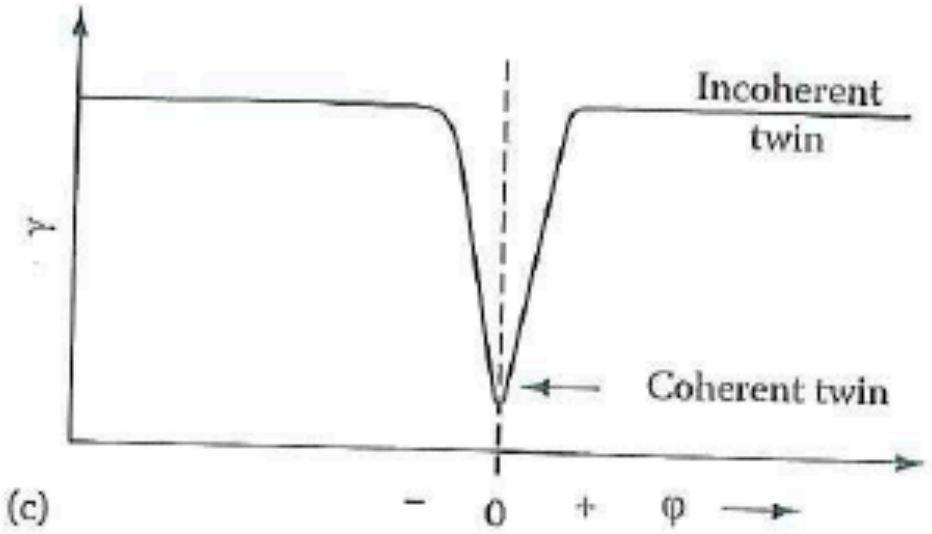
Why are they so straight?



(a)


Incoherent boundary
Twinning plane
Rows of atoms
ϕ

(b)


Incoherent twin
Coherent twin
γ
−
0
+
φ

(c)