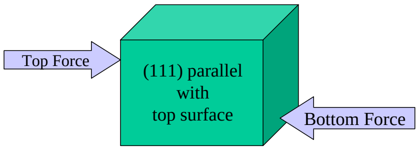
Dislocations in Materials

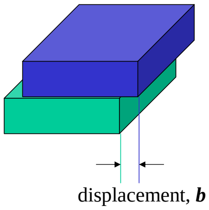
Pose the following case scenario:

- Consider a block of crystalline material on which forces are applied.



Sum of the applied forces give rise to a
Shear Force
on the block of crystalline material.

- Assume the shear force is large enough to cause a displacement, ***b***, of the crystalline material.



Dislocations in Materials

- The displacement occurs between two adjacent (100) slip planes.
- One manner in which the displacement occurs is that the bonds between atoms on adjacent slip planes break and move to the next position.
- If displacement is along atoms A, B, and C, then:
  - ✓ A moves to B site.
  - ✓ B moves to C site, etc.
  - ✓ Simultaneous translation of all atoms on slip plane must occur.
- It seems as though many bonds must be broken simultaneously, considerable energy would be required.
- **Question:** What shear force, τ, would be required to cause this type of displacement?

- **Try To Answer This Question:**
  - ✓ Need to calculate the force required to simultaneously break all the bonds along the slip plane.

Dislocations in Materials

- Compare stresses at which a material yields for:
  - ✓ Theoretical results
  - ✓ Experimental results

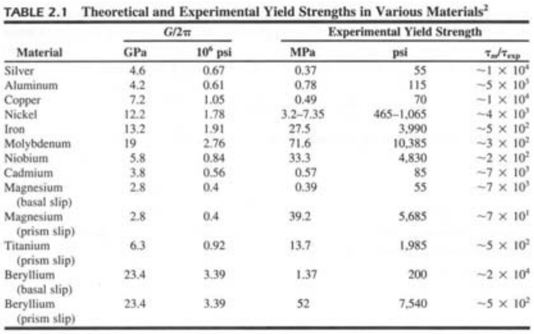


TABLE 2.1 Theoretical and Experimental Yield Strengths in Various Materials[2]

	$G/2\pi$		Experimental Yield Strength		
Material	GPa	10^6 psi	MPa	psi	τ_{th}/τ_{exp}
Silver	4.6	0.67	0.37	55	$\sim 1 \times 10^4$
Aluminum	4.2	0.61	0.78	115	$\sim 5 \times 10^3$
Copper	7.2	1.05	0.49	70	$\sim 1 \times 10^4$
Nickel	12.2	1.78	3.2–7.35	465–1,065	$\sim 4 \times 10^3$
Iron	13.2	1.91	27.5	3,990	$\sim 5 \times 10^2$
Molybdenum	19	2.76	71.6	10,385	$\sim 3 \times 10^2$
Niobium	5.8	0.84	33.3	4,830	$\sim 2 \times 10^2$
Cadmium	3.8	0.56	0.57	85	$\sim 7 \times 10^3$
Magnesium (basal slip)	2.8	0.4	0.39	55	$\sim 7 \times 10^3$
Magnesium (prism slip)	2.8	0.4	39.2	5,685	$\sim 7 \times 10^1$
Titanium (prism slip)	6.3	0.92	13.7	1,985	$\sim 5 \times 10^2$
Beryllium (basal slip)	23.4	3.39	1.37	200	$\sim 2 \times 10^4$
Beryllium (prism slip)	23.4	3.39	52	7,540	$\sim 5 \times 10^2$

- The theoretical stress is much greater than the experimental stress.

What is going on?

Dislocations in Materials

- In 1934, Taylor, Orowan, and Polanyi independently postulated:
- The existence of a *lattice defect* that would allow the block in the previous figure to slip at much lower stress levels.
- The defect they postulated was a *line defect* called a *dislocation*.
- By introducing an extra half plane of atoms into the lattice, they showed:
  - ✓ Atom bond breakage on the slip plane could be restricted to the immediate vicinity of the bottom edge of the half plane = dislocation line.
  - ✓ As dislocation line moves through the x'tal, bond breakage across the slip plane occurs *consecutively* rather than *simultaneously*.
- **Major concept:** takes much less energy to break one bond at a time than all bonds at once.

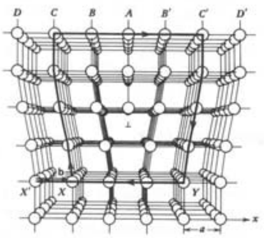


FIGURE 2.3 Lattice defect caused by introduction of an extra half plane of atoms, *A*. Note symmetrical displacement of planes *B*, *B'*, *C*, *C'*, etc. The dislocation line is defined as the edge of the half plane, *A*. The Burgers circuit *XCC'YX'* contains a closure failure *X'X*. (From Guy,[5] *Elements of Physical Metallurgy*, 2nd ed., Addison-Wesley, Reading, MA, 1959.)

Dislocations in Materials

- ❑ **Analogy of the concept of a dislocation:**
  - ✓ Simultaneous bond breaking ~ moving a large floor rug across the room by just pulling.
  - ✓ Consecutive bond breaking ~ shake edge of rug up and down creating a ripple effect – the ripples propagate from one end of the rug to the other end.

Much easier to move rug in this manner

- ❑ This is shown below:

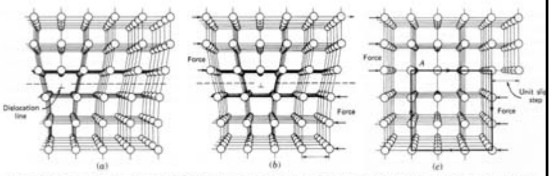


FIGURE 2.4 Successive positions of dislocation as it moves through crystal. Note that the final offset of crystal resulting from the passage of dislocation is the same as the simultaneous movement of the entire crystal. Note the perfect Burgers circuit in (*c*). (From Guy,[5] *Elements of Physical Metallurgy,* 2d ed., Addison-Wesley, Reading, MA, 1959.)

Hertzberg, Deformation & Fracture Mechanics of Engineering Materials, 4th Ed. (Wiley, 1996)

Dislocations in Materials

- ❑ The planes on which dislocations move most readily are those of greatest:
  - ✓ Separation
  - ✓ Atomic density

Known as:
Slip Planes

Table 14-1 Slip systems in common crystals[a]

Structure	Examples	Slip plane, slip direction
F.c.c. (*A*1)	Cu, Ag, Au, Ni, Al	$(111)\ [110]$
	*A*1 at elevated temperatures	$(100)\ [10\bar{1}]$
B.c.c. (*A*2)	α-Fe	(110) (112) $[11\bar{1}]$ (123)
	W, Mo, Na at 0.08 to 0.24 T_m	$(112)^b$
	Mo, Na, β-CuZn, at 0.26 to 0.50 T_m	$(110)^b$
	Na, K, at 0.80 T_m	$(123)^b$
	Nb	(101)
C.p.h. (*A*3)	Cd, Be, Te	$(0001)[11\bar{2}0]$
	Zn	$(0001)[11\bar{2}0]$, $(11\bar{2}2)\ [11\bar{2}\bar{3}]$
	Be, Re, Zr	$(10\bar{1}0)[11\bar{2}0]^c$
	Mg[d]	$(0001)[11\bar{2}0]$, $(11\bar{2}2)[10\bar{1}0]$, $(10\bar{1}1)[11\bar{2}0]$
	Ti, Zr, Hf	$(10\bar{1}0)[11\bar{2}0]$, $(10\bar{1}1)[11\bar{2}0]$, $(0001)[11\bar{2}0]$, $(11\bar{2}2)^e$
CsCl type (*B*1)	LiTl, MgTl, AuZn[f]	$(110)[100]$
	AgMg[f]	$(321)[111]$
	β-CuZn	$(110)[111]$
Orthorhombic (*A*20)	α-U	$(010)[100]$; cross slip on (011), (013) (110)
Tetragonal	β-U[g]	$(110)[001]$
Tetragonal (*A*5)	β (white) Sn	$(110)[001]$, $(100)[001]$, $(100)[01\bar{1}]$, $(10\bar{1})[101]$, $(121)[101]$
Rhombohedral (*A*7)	Bi	$(111)[10\bar{1}]$
	Hg	$(11\bar{1})[\bar{1}10]$, $(11\bar{1})[011]^h$
NaCl type (*B*1)	NaCl, AgCl[f]	$(110)[1\bar{1}0]$, (100)

[a] Except as noted otherwise, data are from: Review by R. Maddin and N. K. Chen in "Progress in Metal Physics," vol. 5, p. 53, Interscience, New York, 1954. R. W. K. Honeycomb in "Progress in Materials Science," vol. 9, Pergamon, New York, 1961. C. S. Barrett, "Structure of Metals," 2d ed., McGraw-Hill, New York, 1953.

[b] T_m is the melting temperature in these determinations by E. N. Da C. Andrade and L. C. Tsien. See also A. T. Churchman, *Proc. Roy. Soc.* (*London*), vol. 226A, p. 216, 1954.

[c] In single crystals of c.p.h. Cu-Ge ζ phase, $\{10\bar{1}0\}$ slip has been observed in addition to $\{0001\}$ slip. P. H. Thornton, *Phil. Mag.*, vol. 11, p. 71, 1965.

[d] R. E. Reed-Hill and W. D. Robertson, *Trans. AIME*, vol. 212, p. 256, 1958.

[e] $(11\bar{2}2)$ in Hf reported by R. E. Reed-Hill, private communication, 1964.

[f] A. H. Cottrell in R. Grammel (ed.), "Deformation and Flow in Solids," p. 33, Springer, Berlin, 1956.

[g] A. N. Holden, *Acta Cryst.*, vol. 5, p. 182, 1952.

[h] J. G. Rider and F. Heckscher, *Phil. Mag.*, vol. 13, p. 687, 1966.

Slip Direction is along ***b***

Barret & Massalski, Structure of Metals, 3rd Ed. (Pergamon, 1980)

Slip system = Slip plane + Slip direction

Dislocations in Materials

- ☐ Several Slip Systems shown in TEM micrograph below.
- ☐ Each array is on a slip plane and has a specific slip direction indicating a slip system.

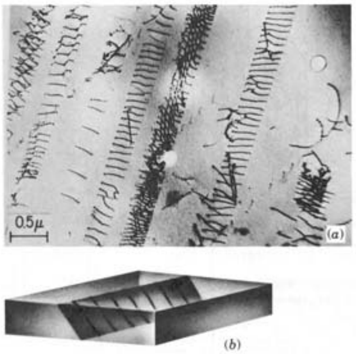


FIGURE 2.13 **Observation of individual dislocations in thin foil. (*a*) Planar arrays of dislocations in 18Cr–8Ni stainless steels (from Michalak,[10] *Metals Handbook*, Vol. 8, copyright American Society for Metals, Metals Park, OH, 1973; used with permission); (*b*) diagram showing position of dislocations on the guide plane in the foil (after Hull[11]).**

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Dislocations in Materials

- ☐ Fundamental characteristics of dislocations:
  - ✓ A dislocation is a lattice line defect.
  - ✓ The *line* or *dislocation* defines the boundary between *slipped* and *unslipped* portions of the crystal.
  - ✓ Dislocations can terminate at:
    - o free surface
    - o boundaries (e.g., grain boundary, interface, etc.).
    - o Another dislocation
  - ✓ Dislocations can never terminate within the crystal.
  - ✓ Consequently, dislocations must either form:

Closed loops

Or:
networks with *branches* that *terminate* at the *surface* or at *boundaries*

Dislocations in Materials

- ❑ Dislocations are described by two vectors
  - ✓ ***b*** = Burgers vector
  - ✓ ***l*** = dislocation line vector is the vector that designates the line of broken bonds that moves through the crystal.

Burgers vector circuit:

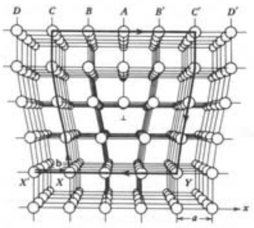

FIGURE 2.3 Lattice defect caused by introduction of an extra half plane of atoms, *A*. Note symmetrical displacement of planes *B*, *B′*, *C*, *C′*, etc. The dislocation line is defined as the edge of the half plane, *A*. The Burgers circuit *XCC′YX′* contains a closure failure *X′X*. (From Guy,[5] *Elements of Physical Metallurgy*, 2nd ed., Addison-Wesley, Reading, MA, 1959.)

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Dislocations in Materials

- ❑ Types of Dislocations:
  - ✓ Edge
  - ✓ Screw
  - ✓ Mixed
  - ✓ Perfect, Pure, Whole
  - ✓ Partial

TABLE 2.4 Characteristics of Dislocations

	Type of Dislocation	
Dislocation Characteristic	**Edge**	**Screw**
Slip direction	Parallel to **b**	Parallel to **b**
Relation between dislocation line and **b**	Perpendicular	Parallel
Direction of dislocation line movement relative to **b**	Parallel	Perpendicular
Process by which dislocations may leave the glide plane	Nonconservative climb	Cross-slip

- ❑ Edge Dislocation:

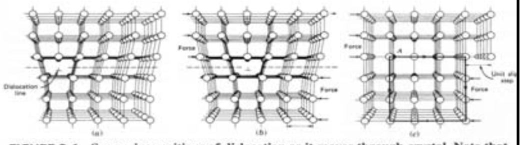

FIGURE 2.4 Successive positions of dislocation as it moves through crystal. Note that the final offset of crystal resulting from the passage of dislocation is the same as the simultaneous movement of the entire crystal. Note the perfect Burgers circuit in (*c*). (From Guy,[5] *Elements of Physical Metallurgy*, 2d ed., Addison-Wesley, Reading, MA, 1959.)

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Dislocations in Materials

☐ Screw dislocation:

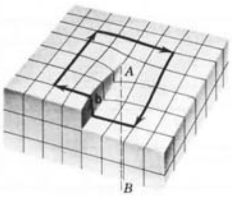

FIGURE 2.8 Screw dislocation *AB* resulting from displacement of one part of crystal relative to the other. Note that *AB* is parallel to b.

☐ Mixed dislocation:

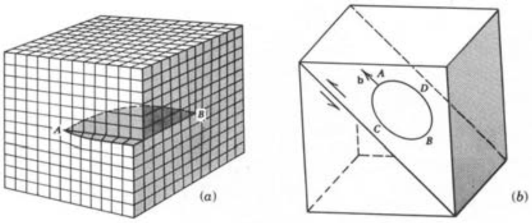

FIGURE 2.10 Curved dislocations containing edge and screw components. (*a*) Dislocation *AB* is pure screw at *A* and pure edge at *B*; (*b*) dislocation loop that grows out radially with shear stress applied parallel to b.

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Dislocations in Materials

☐ Dislocation Motion:

- ✓ Edge Dislocations:
  - o Conservative:
    - Motion inside the slip system.
    - Mass is conserved (diffusion to or from dislocation not required).
    - This motion is known as ***GLIDE***.
  - o Nonconservative:
    - Motion outside the normal slip plane.
    - Mass is not conserved.
    - Thus, vacancies or atoms must be consumed in order for motion to occur.
    - This motion is known as ***CLIMB***.

Dislocation Climb

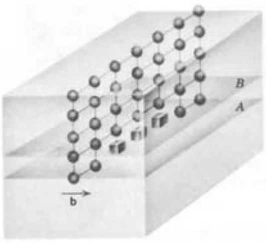

FIGURE 2.7 Dislocation climb involving vacancy (□) diffusion to edge dislocation allowing its movement to climb from plane *A* to plane *B*.

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Dislocations in Materials

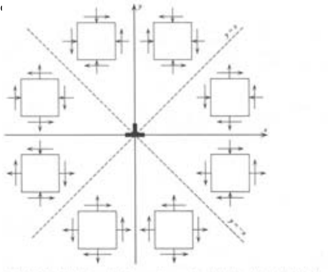

FIGURE 2.15 Elastic stress field surrounding an edge dislocation. (From Read,[3] *Dislocations in Crystals;* copyright McGraw-Hill Book Co., New York, © 1953. Used with permission of McGraw-Hill Book Company.)

Stress Field
Around a
Dislocation

- ❑ Dislocation interaction due to Stress Field:
  - ✓ Edge-Edge
  - ✓ Edge-Screw
  - ✓ Screw-Screw
- ❑ Dislocations on same slip plane:
  - ✓ Dislocations of the same sign will repel one another.
    - o Dislocation pile-up can occur.
    - o This results in a large stress concentration at the leading edge of the pile up.
    - o This can lead to premature fracture of material.
  - ✓ Dislocation of opposite sign will attract one another.

Driving force = **stress field**

- ❑ Dislocations on dissimilar slip planes:
  - ✓ Interaction will occur.
  - ✓ Motion may be impeded.

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Dislocations in Materials

- ❑ Dislocation Strain Energy:
  - ✓ Magnitude of stored energy in an elastically strained region is always of the form:

$$\text{Strain Energy} = \frac{1}{2}\cdot(\text{elastic modulus})\cdot(\text{strain})^2$$

  - ✓ Strain at any given point is proportional to ***b***.
  - ✓ Thus, Elastic Strain Energy is proportional to ***b*²**.

$$E_{screw} = \frac{Gb^2}{4\pi}\ln\left(\frac{r_{outer}}{r_{inner}}\right)$$

$$E_{edge} = \frac{Gb^2}{4\pi(1-\nu)}\ln\left(\frac{r_{outer}}{r_{inner}}\right)$$

$$E_{mixed} = \frac{Kb^2}{4\pi(1-\nu)}\ln\left(\frac{r_{outer}}{r_{inner}}\right)$$

Key concept:

$$E_{elastic} \propto b^2$$

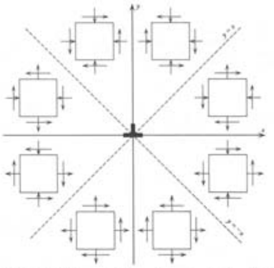

FIGURE 2.15 Elastic stress field surrounding an edge dislocation. (From Read,[3] *Dislocations in Crystals;* copyright McGraw-Hill Book Co., New York, © 1953. Used with permission of McGraw-Hill Book Company.)

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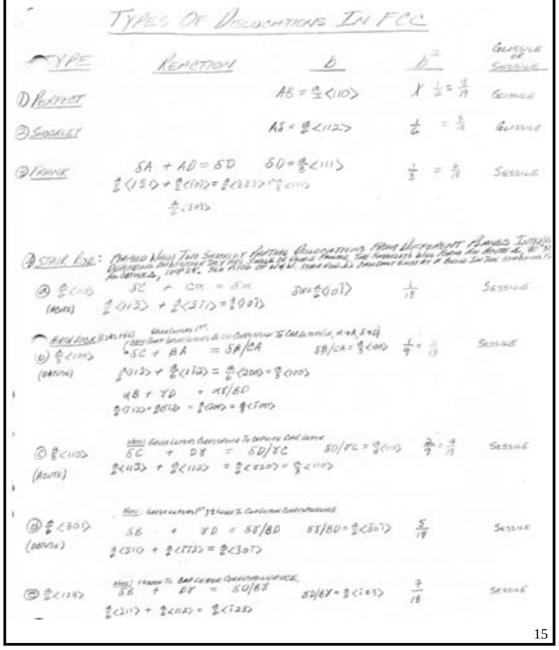
Defects in Semiconductors

- ❑ Partial Dislocations:



TYPES OF DISLOCATIONS IN FCC

TYPE	REACTION	b	b^2	GLISSILE OR SESSILE
① PERFECT		$AB = \frac{a}{2}\langle 110\rangle$	$\frac{1}{2} = \frac{9}{18}$	GLISSILE
② SHOCKLEY		$A\delta = \frac{a}{6}\langle 112\rangle$	$\frac{1}{6} = \frac{3}{18}$	GLISSILE
③ FRANK	$\delta A + AD = \delta D$ $\frac{a}{6}\langle 1\bar{2}1\rangle + \frac{a}{2}\langle \bar{1}01\rangle = \frac{a}{6}\langle \bar{2}\bar{2}\bar{2}\rangle = \frac{a}{3}\langle 111\rangle$ $\frac{a}{6}\langle 301\rangle$	$\delta D = \frac{a}{3}\langle 111\rangle$	$\frac{1}{3} = \frac{6}{18}$	SESSILE

④ STAIR ROD: FORMED WHEN TWO SHOCKLEY PARTIAL DISLOCATIONS FROM DIFFERENT PLANES INTERSECT [illegible]

TYPE	REACTION	b	b^2	GLISSILE OR SESSILE
ⓐ $\frac{a}{6}\langle 110\rangle$ (ACUTE)	$\delta C + C\alpha = \delta\alpha$ $\frac{a}{6}\langle 11\bar{2}\rangle + \frac{a}{6}\langle \bar{2}\bar{1}1\rangle = \frac{a}{6}\langle \bar{1}0\bar{1}\rangle$	$\delta\alpha = \frac{a}{6}\langle 10\bar{1}\rangle$	$\frac{1}{18}$	SESSILE
ⓑ $\frac{a}{3}\langle 100\rangle$ (OBTUSE)	[illegible] $\delta C + \beta A = \delta\beta/CA$ $\frac{a}{6}\langle 112\rangle + \frac{a}{6}\langle 1\bar{1}\bar{2}\rangle = \frac{a}{6}\langle 200\rangle = \frac{a}{3}\langle 100\rangle$ $\alpha B + \gamma D = \alpha\gamma/BD$ $\frac{a}{6}\langle \bar{1}12\rangle + \frac{a}{6}\langle \bar{1}\bar{1}\bar{2}\rangle = \frac{a}{6}\langle 200\rangle = \frac{a}{3}\langle \bar{1}00\rangle$	$\delta\beta/CA = \frac{a}{3}\langle 100\rangle$	$\frac{1}{9} = \frac{2}{18}$	SESSILE
ⓒ $\frac{a}{3}\langle 110\rangle$ (ACUTE)	[illegible] $\delta C + D\gamma = \delta D/\gamma C$ $\frac{a}{6}\langle 11\bar{2}\rangle + \frac{a}{6}\langle 112\rangle = \frac{a}{6}\langle 220\rangle = \frac{a}{3}\langle 110\rangle$	$\delta D/\gamma C = \frac{a}{3}\langle 110\rangle$	$\frac{2}{9} = \frac{4}{18}$	SESSILE
ⓓ $\frac{a}{6}\langle 301\rangle$ (OBTUSE)	[illegible] $\delta B + \gamma D = \delta\gamma/BD$ $\frac{a}{6}\langle 211\rangle + \frac{a}{6}\langle \bar{1}\bar{1}\bar{2}\rangle = \frac{a}{6}\langle 30\bar{1}\rangle$	$\delta\gamma/BD = \frac{a}{6}\langle \bar{3}0\bar{1}\rangle$	$\frac{5}{18}$	SESSILE
ⓔ $\frac{a}{6}\langle 123\rangle$	[illegible] $\delta B + D\gamma = \delta D/B\gamma$ $\frac{a}{6}\langle 211\rangle + \frac{a}{6}\langle 112\rangle = \frac{a}{6}\langle \bar{1}23\rangle$	$\delta D/B\gamma = \frac{a}{6}\langle \bar{1}23\rangle$	$\frac{7}{18}$	SESSILE