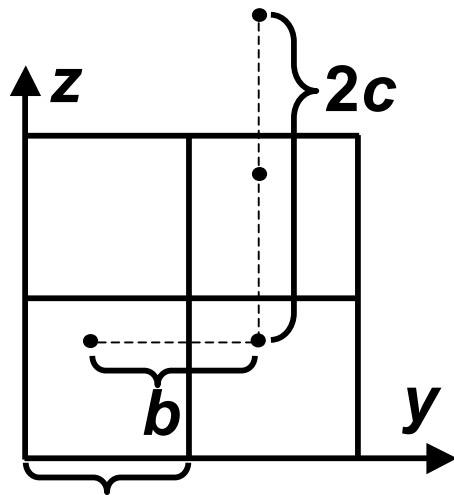
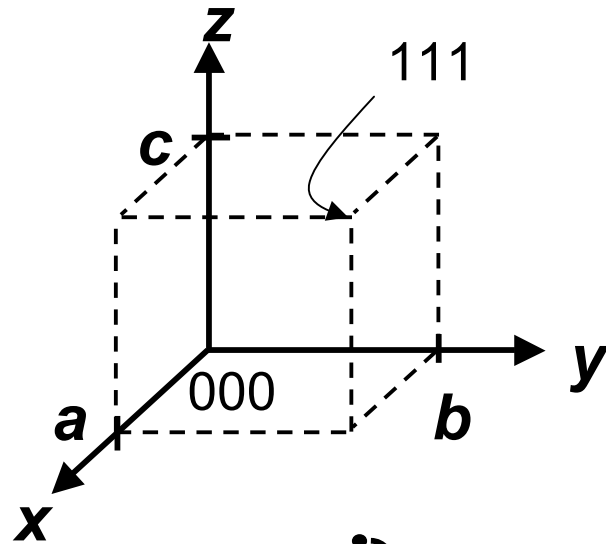
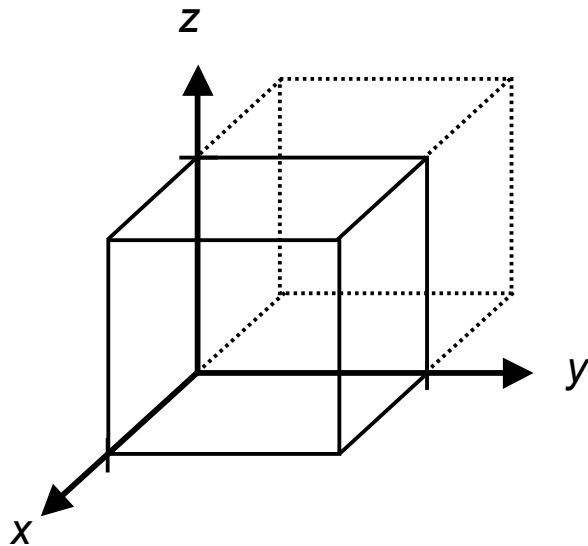


Point coordinates



Point coordinates



Algorithm

1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions a , b , and c
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas
[xyz]

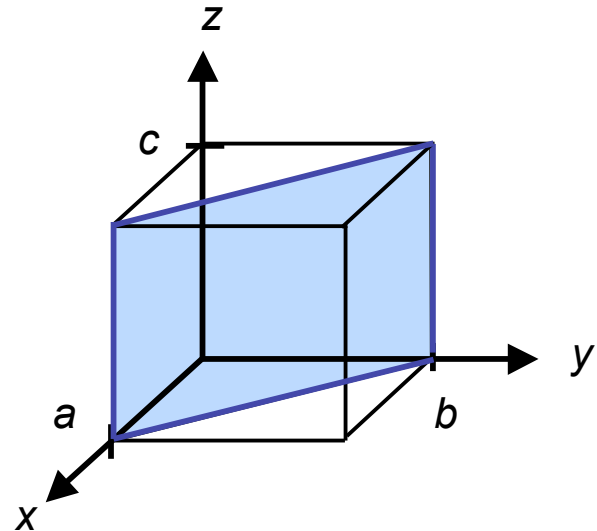
Crystallographic planes

Miller Indices: Reciprocals of the (three) axial intercepts for a plane, cleared of fractions & common multiples. All parallel planes have same Miller indices.

Algorithm

example

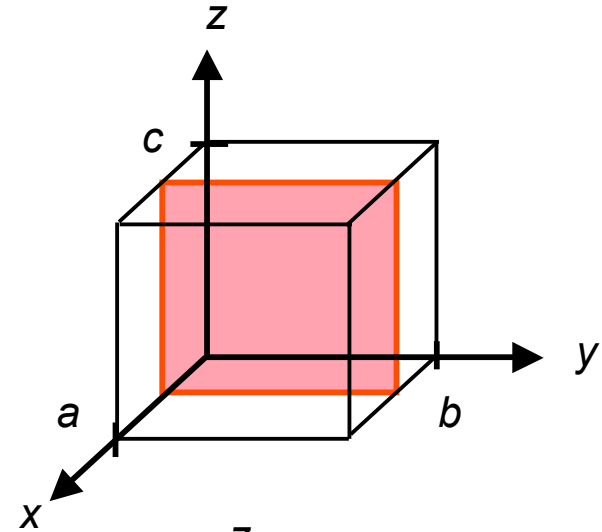
a b c



Crystallographic planes

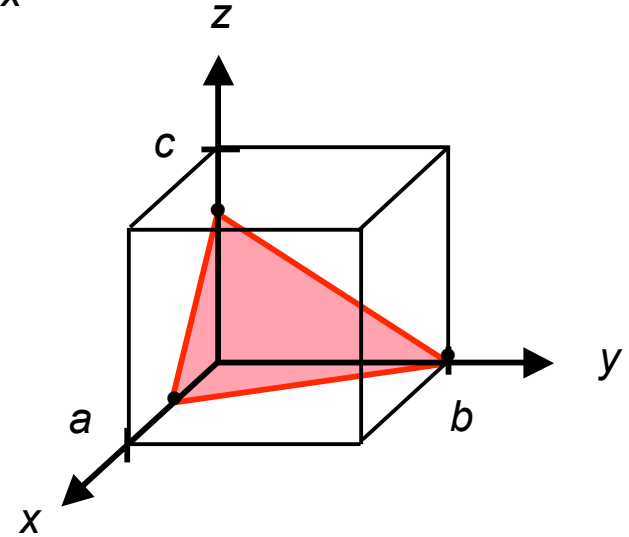
example

a b c



example

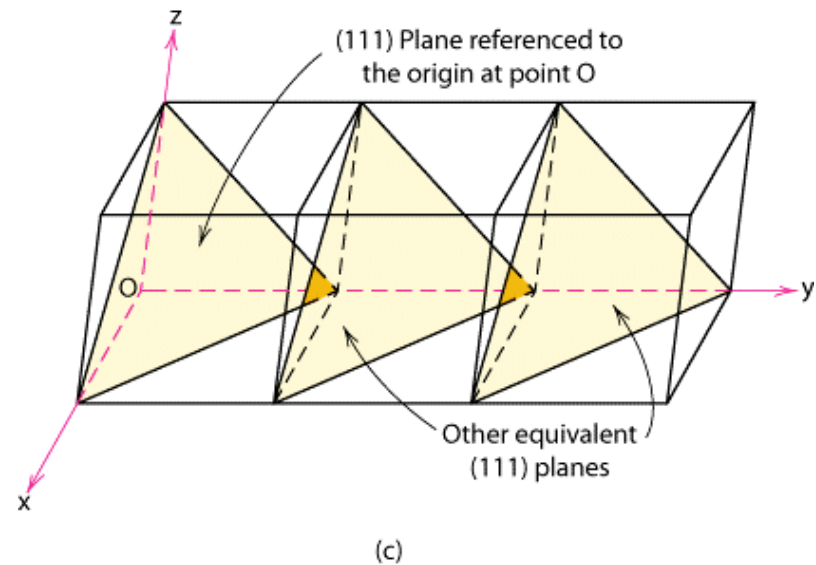
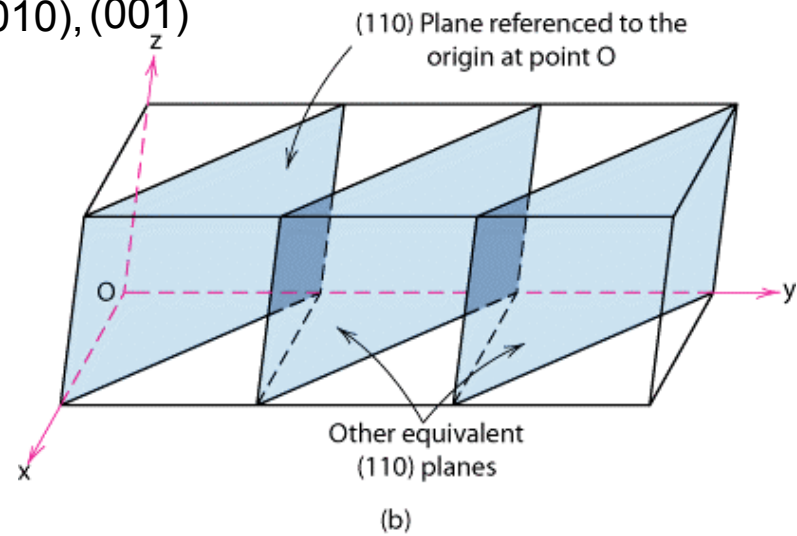
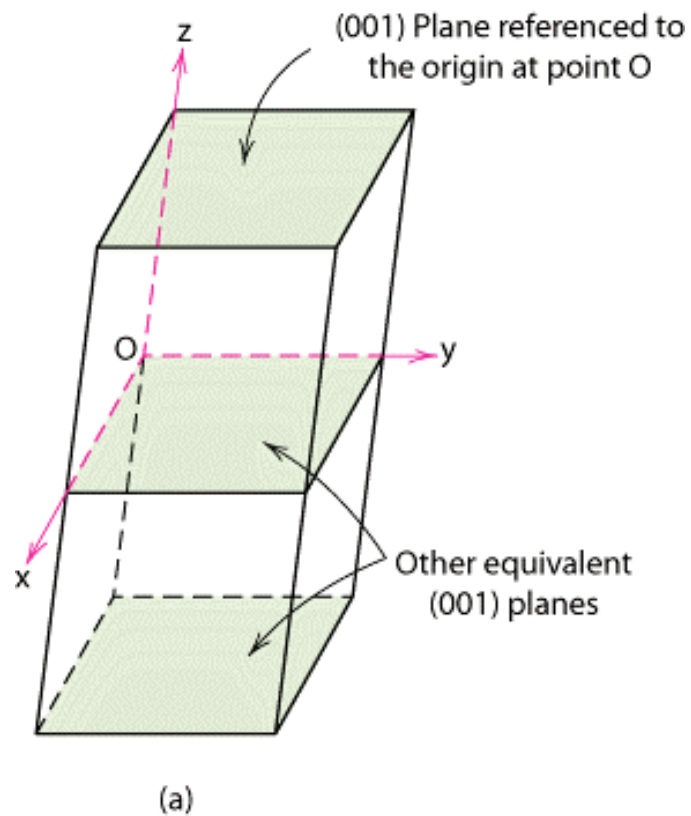
a b c



Crystallographic planes

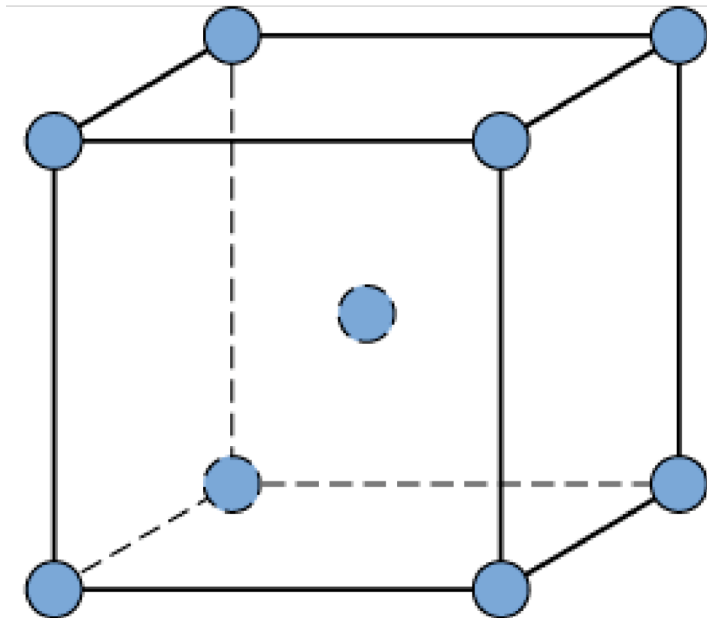
Family of Planes $\{hkl\}$

Ex: $\{100\} = (100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1})$

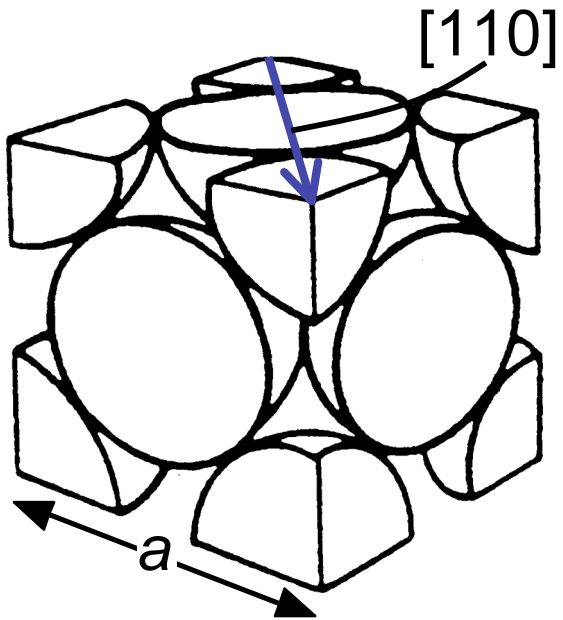


Adapted from Fig. 3.9, *Callister 7e*.

Linear density: BCC

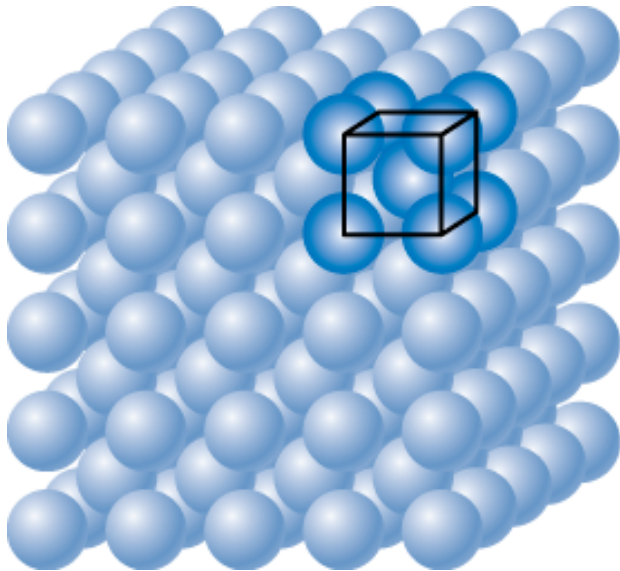


Linear density (FCC) and planar density



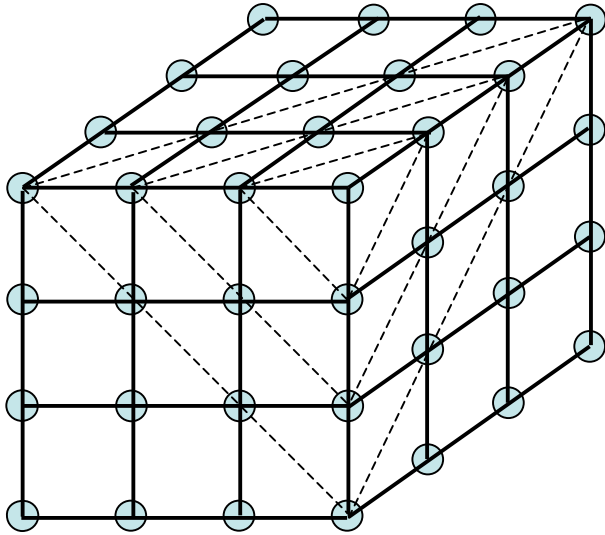
Planar density

- We want to examine the atomic packing of crystallographic planes
 - Iron foil can be used as a catalyst. The atomic packing of the exposed planes is important.
 - a) Draw (100) and (111) crystallographic planes for Fe.
 - b) Calculate the planar density for each of these planes.
- $R = 0.1241 \text{ nm}$ and Fe has a BCC structure at room temperature



Adapted from Fig. 3.2(c), *Callister 7e*.

Planar density



Single crystal vs. Polycrystalline structures

Single crystals: Atoms all have the same arrangement throughout.

Polycrystalline: Many crystals put together.



Anisotropic

Adapted from Fig. K,
color inset pages of
Callister 5e.
(Fig. K is courtesy of
Paul E. Danielson,
Teledyne Wah Chang
Albany)

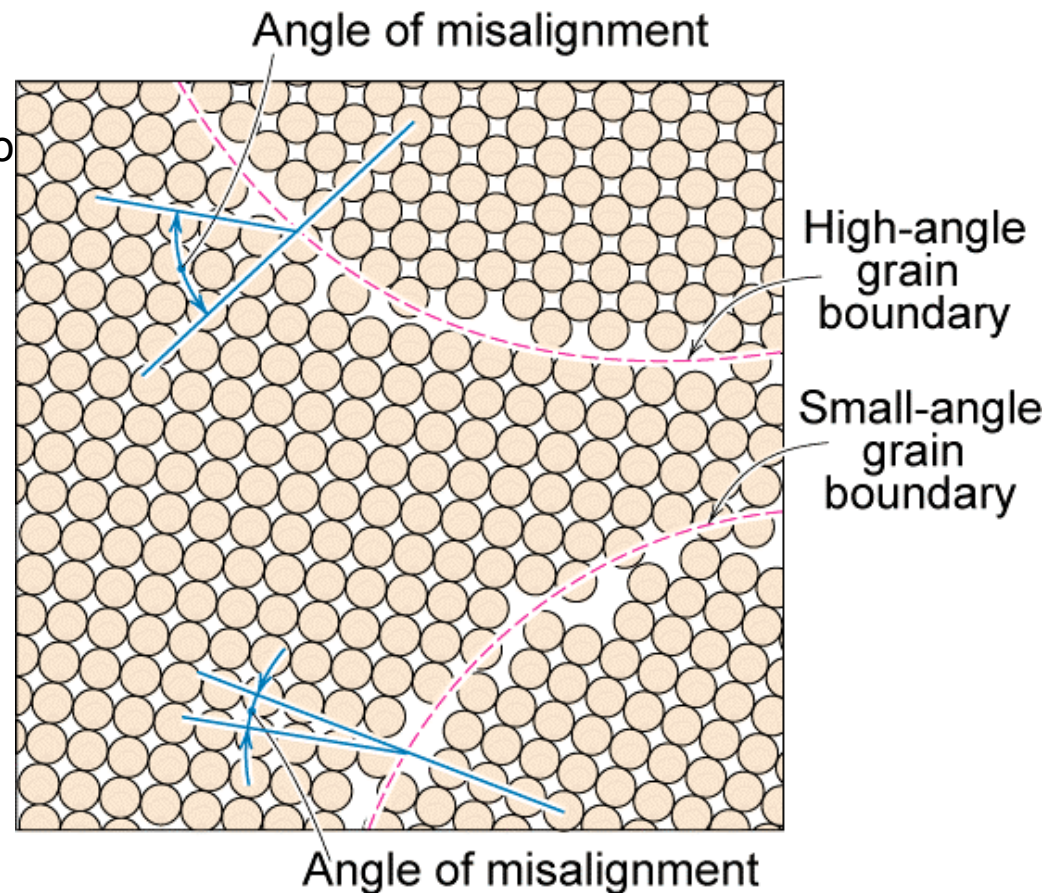
Isotropic

- Nb-Hf-W plate with an electron beam weld.
- Each "grain" is a single crystal.
- If grains are randomly oriented,
overall component properties are not directional.
- Grain sizes typ. range from 1 nm to 2 cm
(i.e., from a few to millions of atomic layers).

Polycrystalline structures

Grain Boundaries

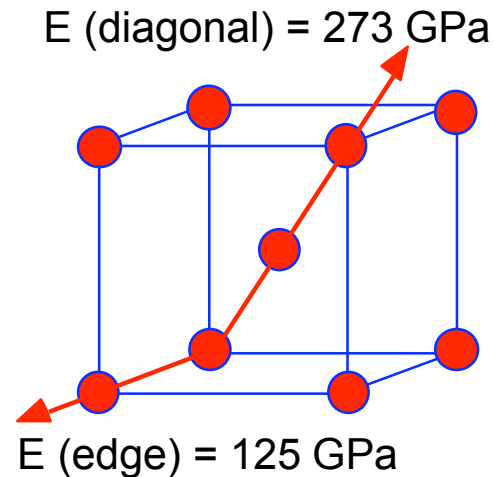
- regions between crystals
- transition from lattice of one region to that of the other
- slightly disordered
- low density in grain boundaries
 - o high mobility
 - o high diffusivity
 - o high chemical reactivity



Adapted from Fig. 4.7, *Callister 7e*.

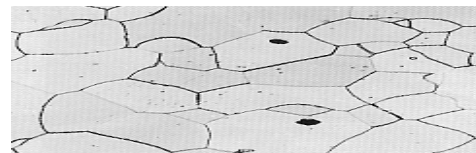
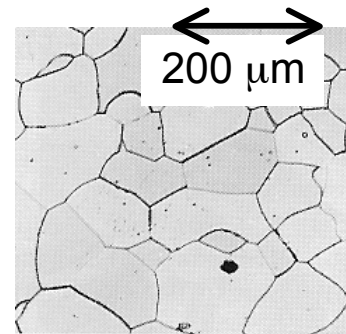
Single crystal vs. Polycrystalline structures

- Single Crystals



Data from Table 3.3, *Callister 7e*.
(Source of data is R.W. Hertzberg, *Deformation and Fracture Mechanics of Engineering Materials*, 3rd ed., John Wiley and Sons, 1989.)

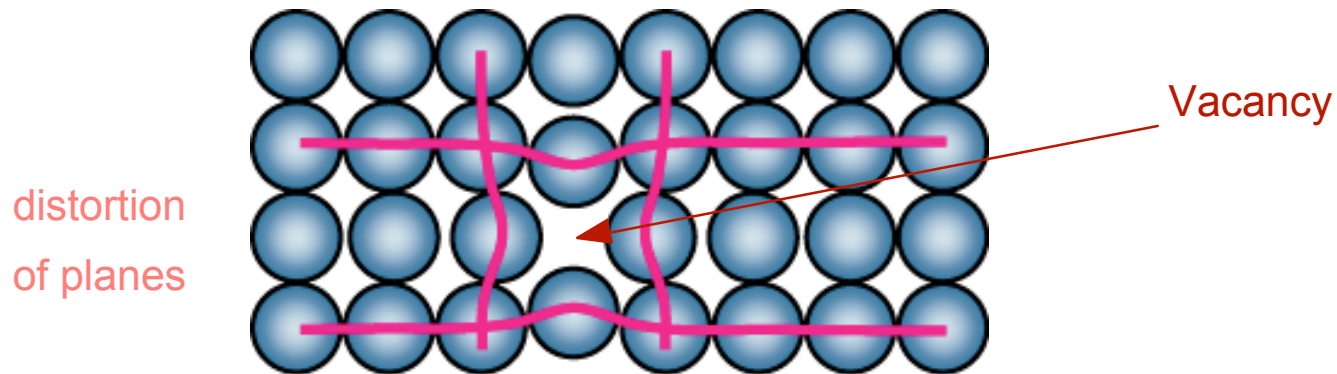
- Polycrystals



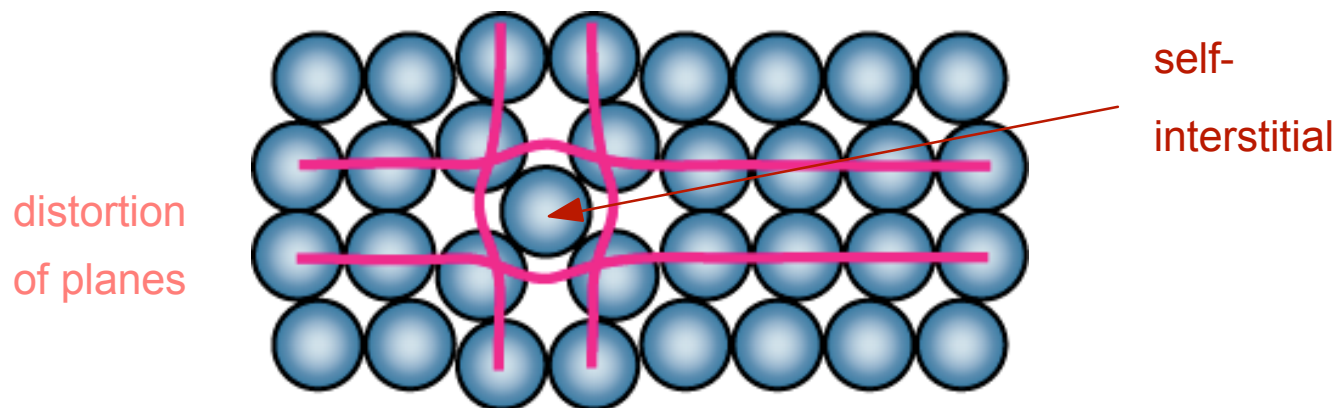
Adapted from Fig. 4.14(b), *Callister 7e*.
(Fig. 4.14(b) is courtesy of L.C. Smith and C. Brady, the National Bureau of Standards, Washington, DC [now the National Institute of Standards and Technology, Gaithersburg, MD].)

Point defects

- Vacancies:
 - vacant atomic sites in a structure.

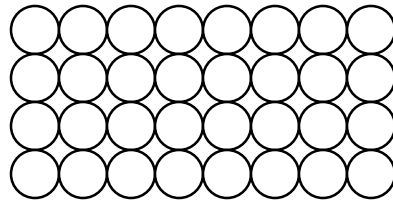


- Self-Interstitials:
 - "extra" atoms positioned between atomic sites.



Equilibrium concentration of defects

- Equilibrium concentration varies with temperature



Each lattice site is a potential vacancy

$$\frac{N_v}{N} = \exp \left(\frac{-Q_v}{kT} \right)$$

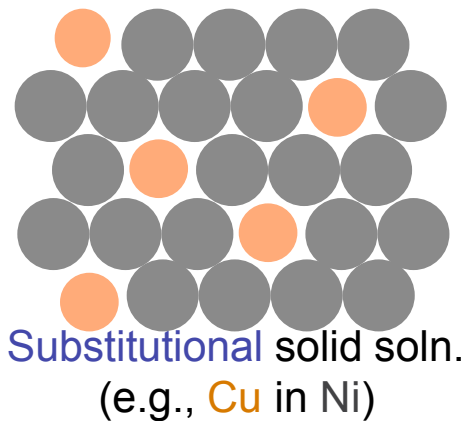
Diagram illustrating the equation for the equilibrium concentration of defects:

- No. of defects** (blue text) points to N_v .
- No. of potential defect sites.** (black text) points to N .
- Activation energy** (red text) points to Q_v .
- Boltzmann's constant** (green text) points to k .
- Temperature** (yellow text) points to T .

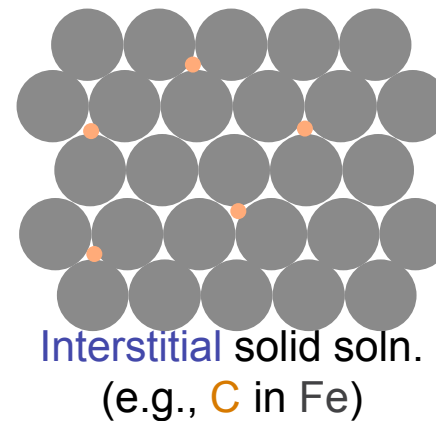
Point defects in alloys

Two outcomes if impurity (B) added to host (A):

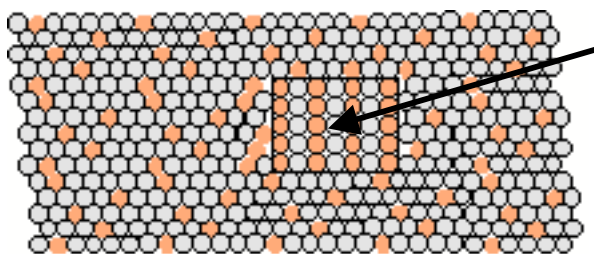
- Solid solution of B in A (i.e., random dist. of point defects)



OR



- Solid solution of B in A plus particles of a new phase (usually for a larger amount of B)



Second phase particle
--different composition
--often different structure.

Imperfections of solids

Conditions for substitutional solid solution (S.S.)

W. Hume – Rothery rule

1. Δr (atomic radius) < 15%
2. Proximity in periodic table
i.e., similar electronegativities
3. Same crystal structure for pure metals
4. Valency

All else being equal, a metal will have a greater tendency to dissolve a metal of higher valency than one of lower valency

1. Would you predict more Al or Ag to dissolve in Zn?
2. More Zn or Al in Cu?

Table on p. 106, *Callister 7e*.

<i>Element</i>	<i>Atomic Radius (nm)</i>	<i>Crystal Structure</i>	<i>Electro- nega- tivity</i>	<i>Valence</i>
Cu	0.1278	FCC	1.9	+2
C	0.071			
H	0.046			
O	0.060			
Ag	0.1445	FCC	1.9	+1
Al	0.1431	FCC	1.5	+3
Ni	0.1246	FCC	1.8	+2
Zn	0.1332	HCP	1.6	+2

Line defects

- Linear Defects (**Dislocations**)
 - Are one-dimensional defects around which atoms are misaligned
- **Edge dislocation**:
 - extra half-plane of atoms inserted in a crystal structure
 - $\mathbf{b} \perp$ to dislocation line
- **Screw dislocation**:
 - spiral planar ramp resulting from shear deformation
 - $\mathbf{b} \parallel$ to dislocation line

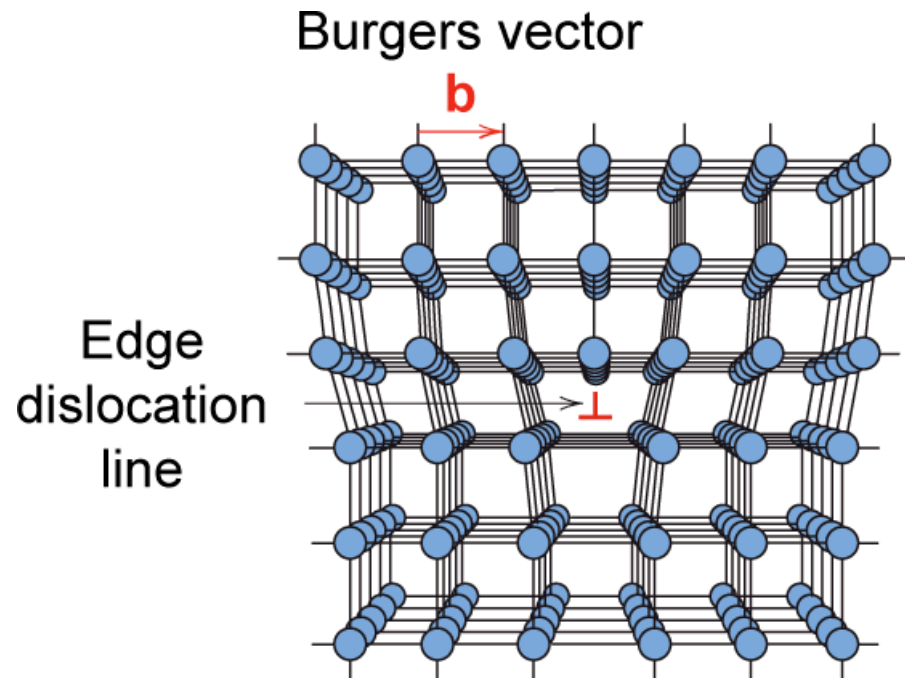
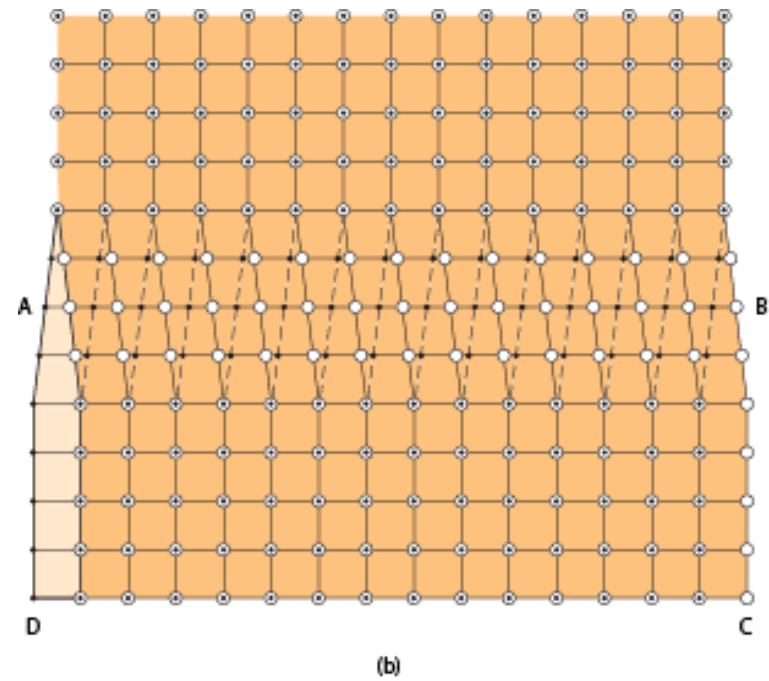
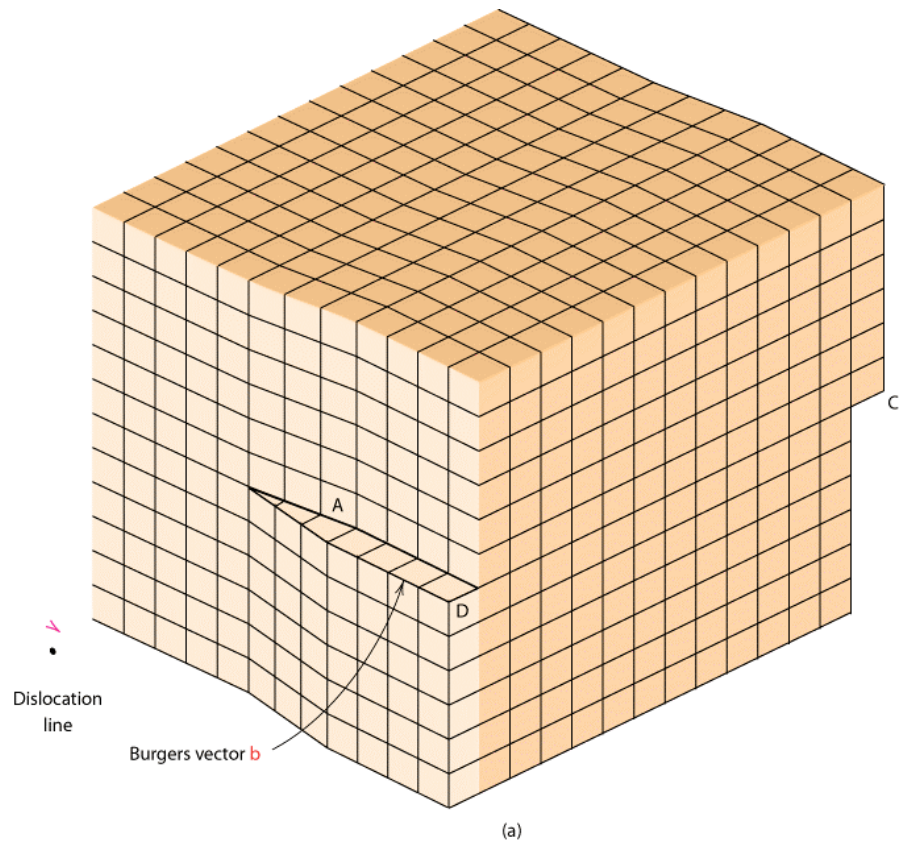


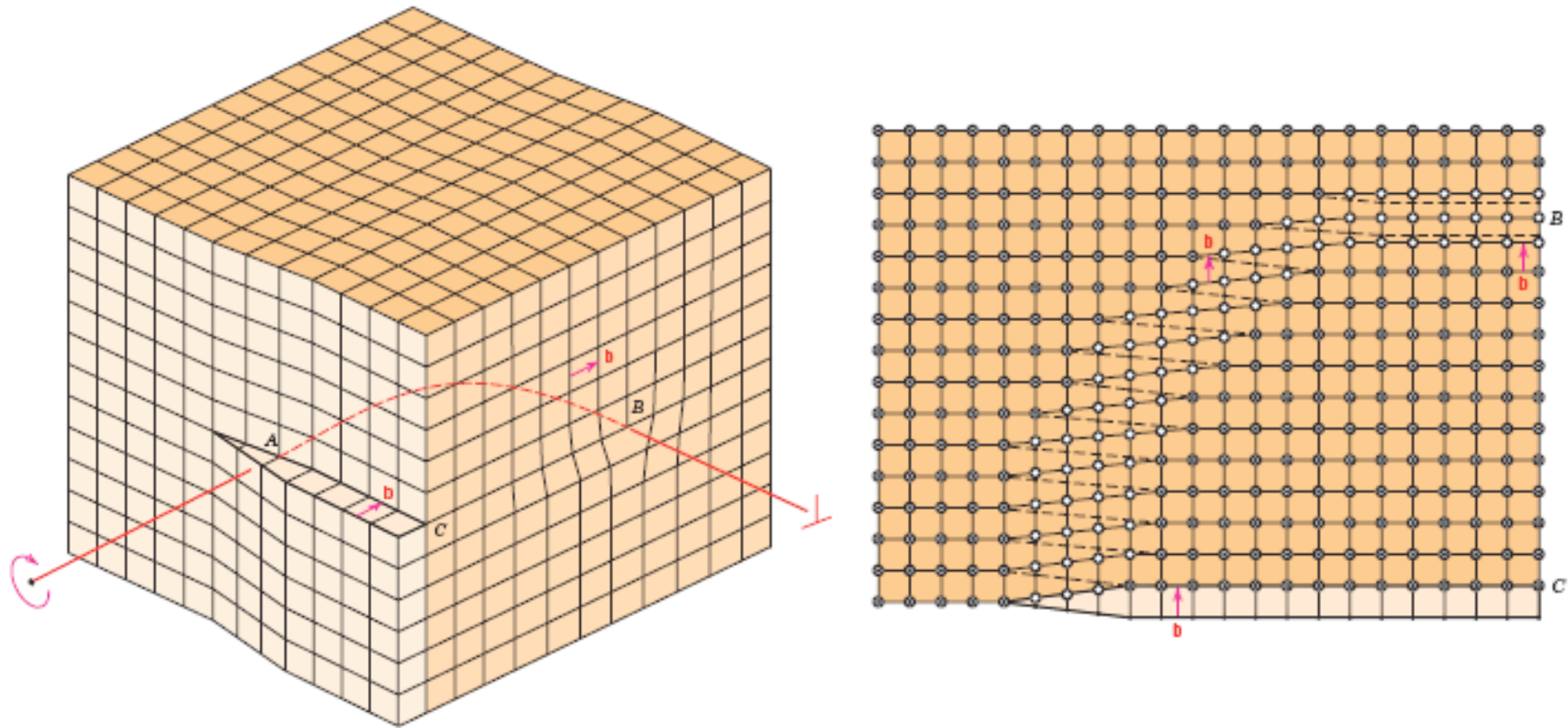
Fig. 4.3, Callister 7e.

Screw defects



Adapted from Fig. 4.4, *Callister 7e*.

Mixed defects

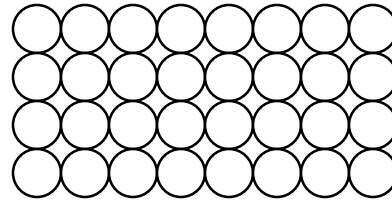


Adapted from Fig. 4.5, *Callister 7e*.

Planar defects

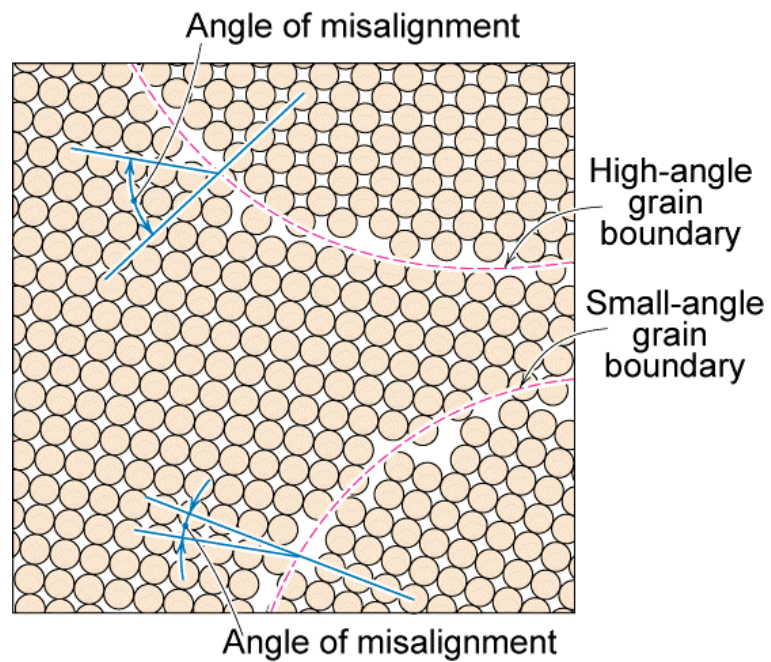
- External defects

- On the surface
- Unsatisfied bonds



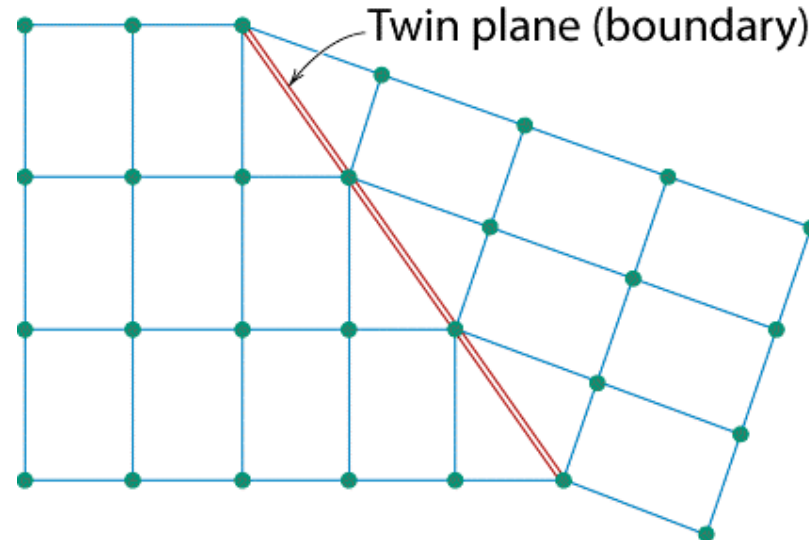
- Internal defects

- Grain boundaries



Planar defects

- Twin boundary (plane)
Essentially a reflection of atom positions across the **twin plane**.



Adapted from Fig. 4.9, *Callister 7e*.

- Stacking faults
For FCC metals an error in ABCABC packing sequence
Ex: ABCABABC