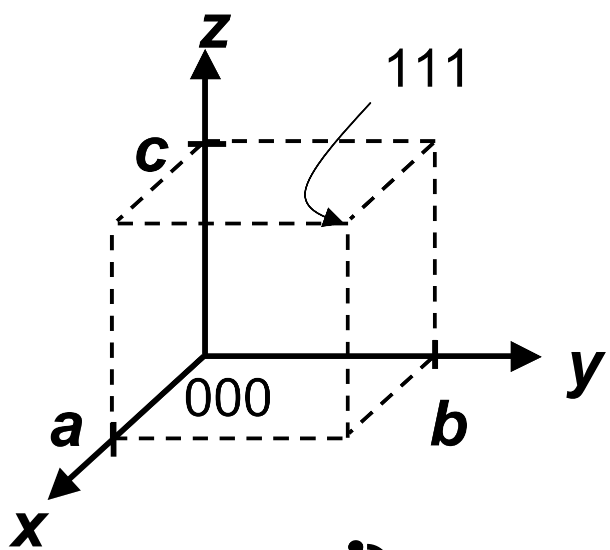
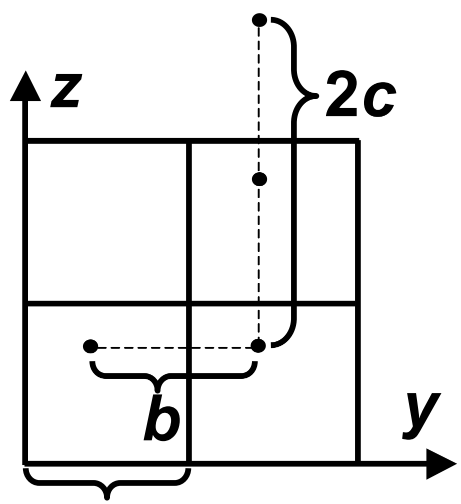
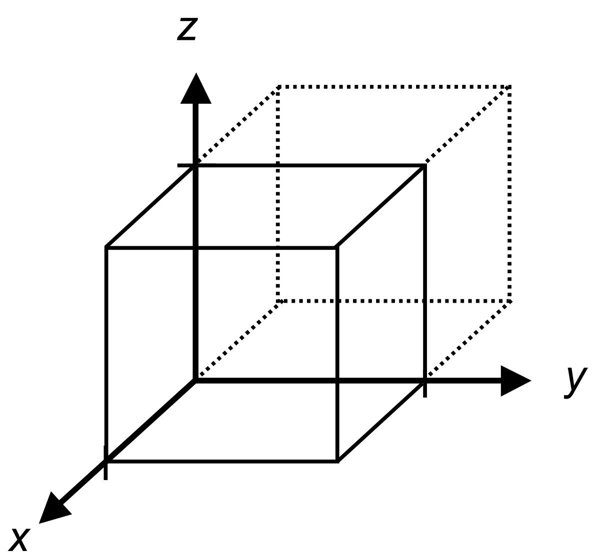
Point coordinates





Point coordinates



Algorithm

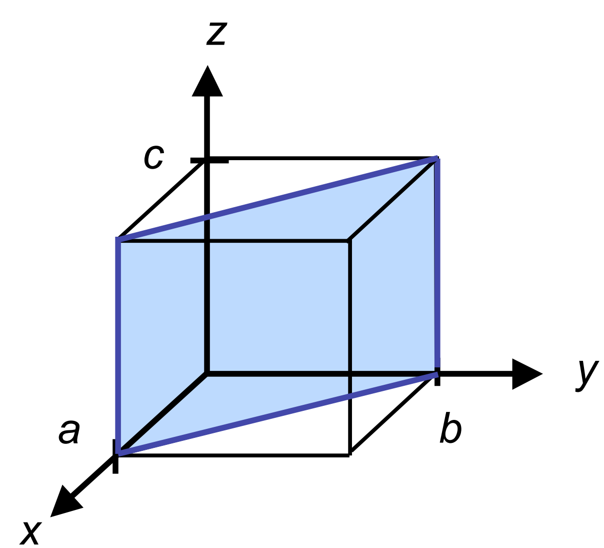
1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions *a*, *b*, and *c*
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas
   [*xyz*]

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

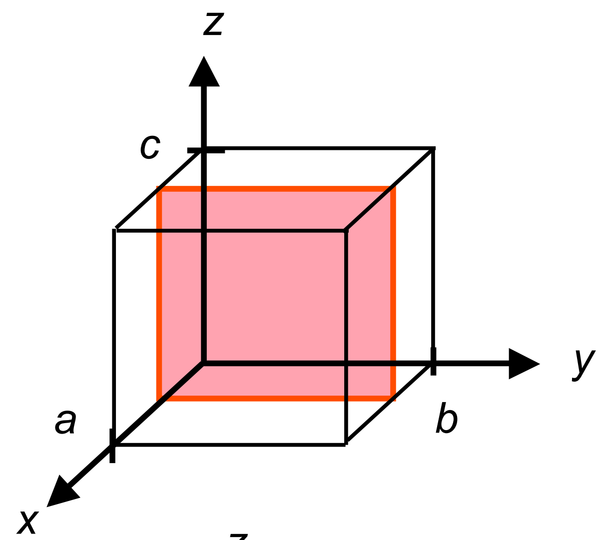
<u>example</u> a b c



Crystallographic planes

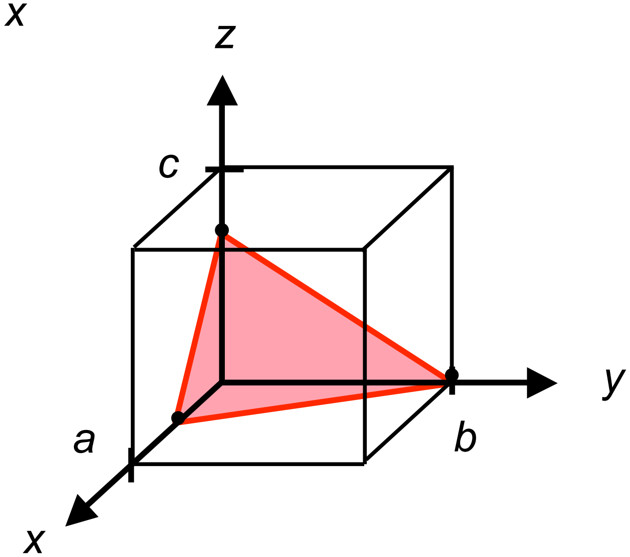
<u>example</u>

a *b* *c*



<u>example</u>

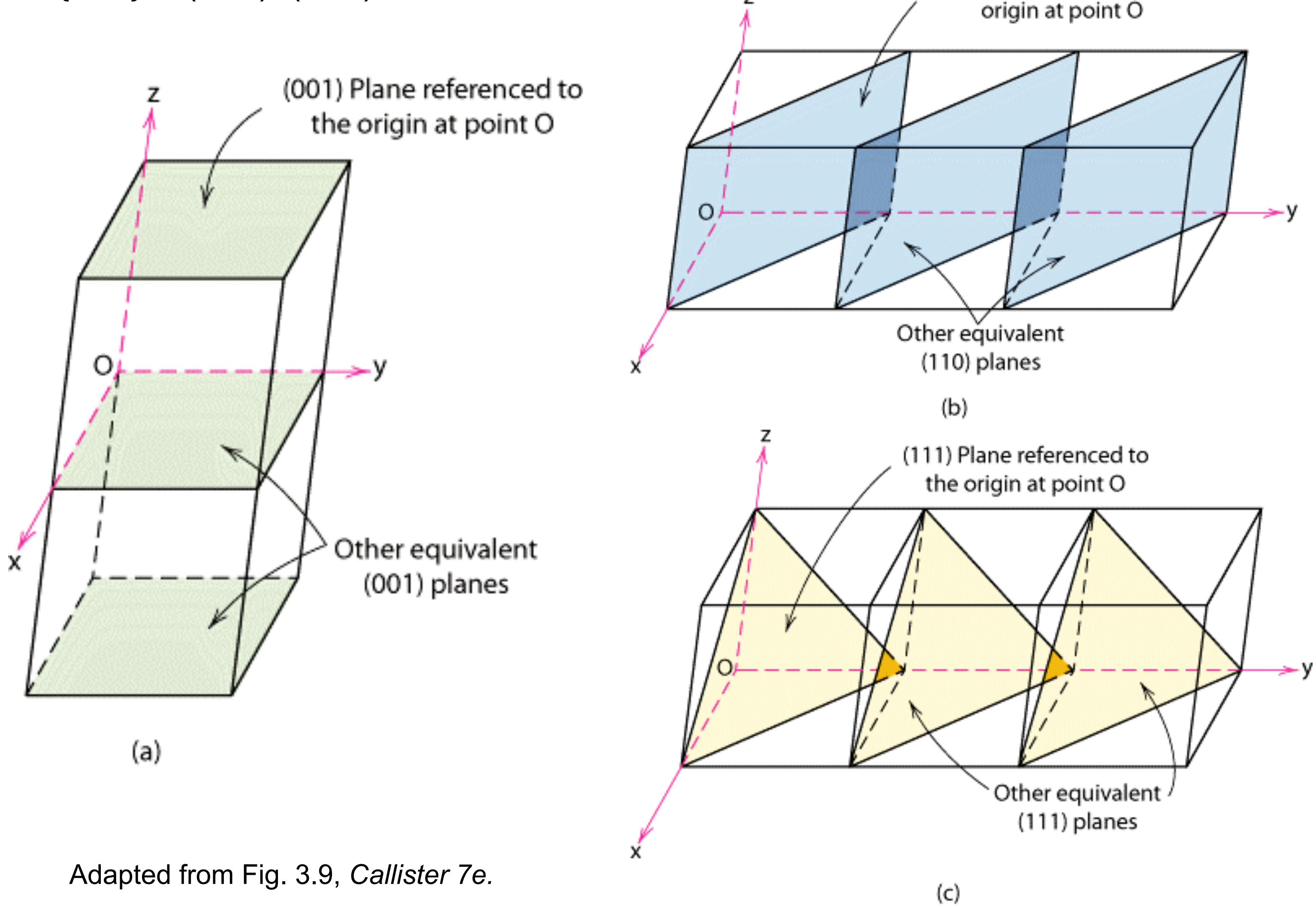
a *b* *c*



Crystallographic planes

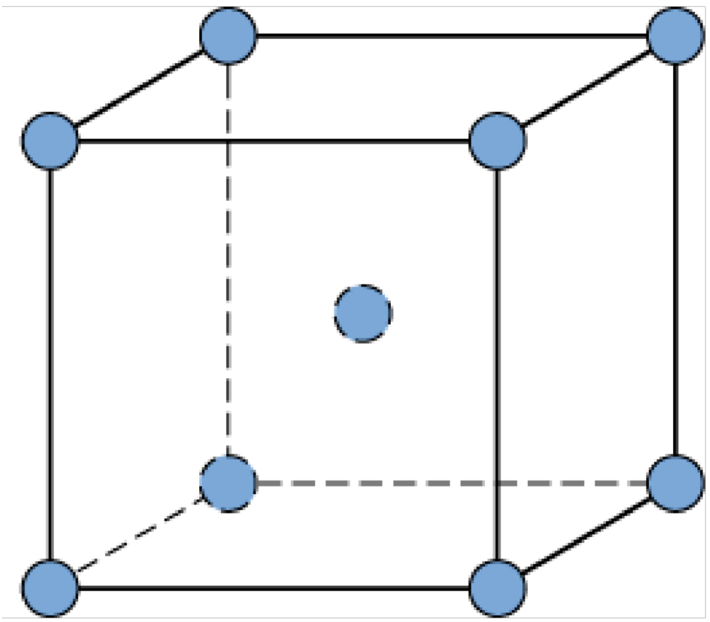
Family of Planes {*hkl*}

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

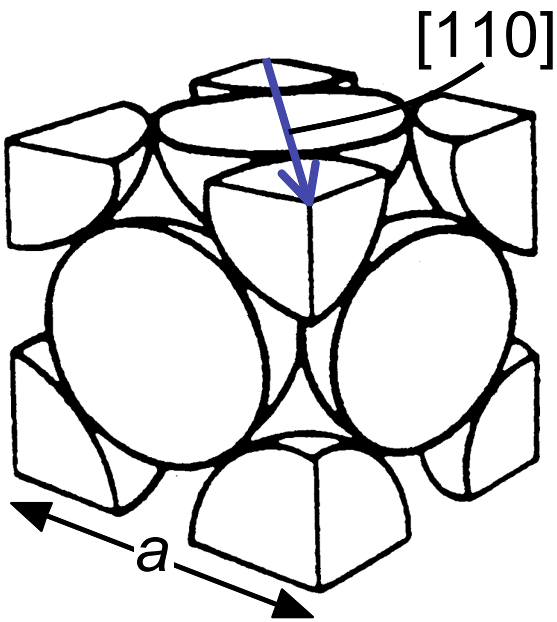


Adapted from Fig. 3.9, *Callister 7e.*

Linear density: BCC



Linear density (FCC) and planar densitry



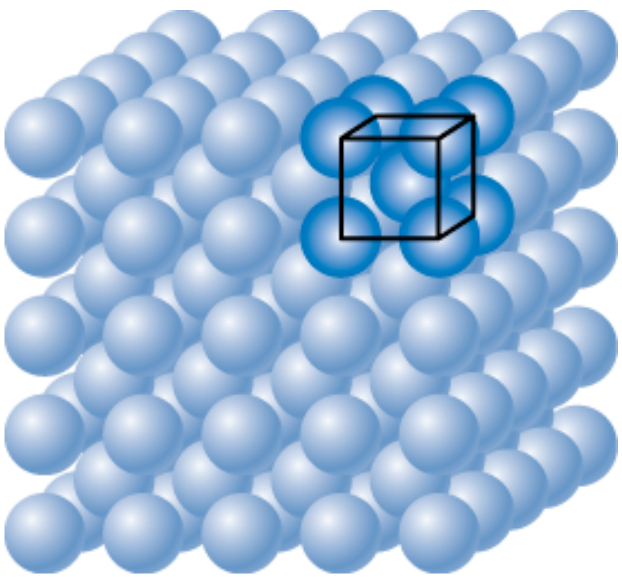
Planar density

- 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.

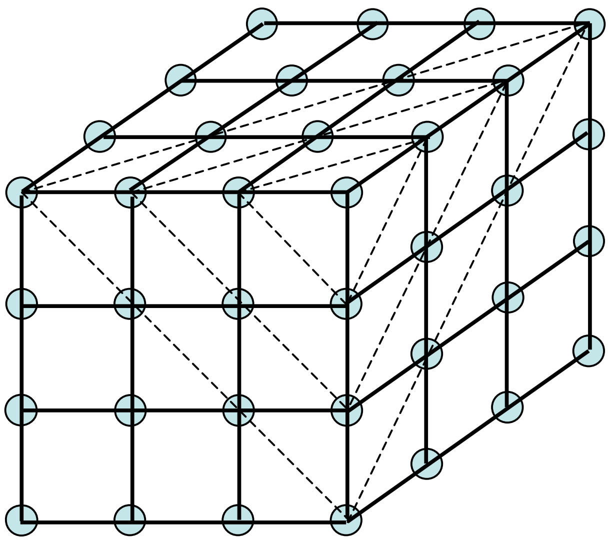
  b) Calculate the planar density for each of these planes.

  R = 0.1241 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)

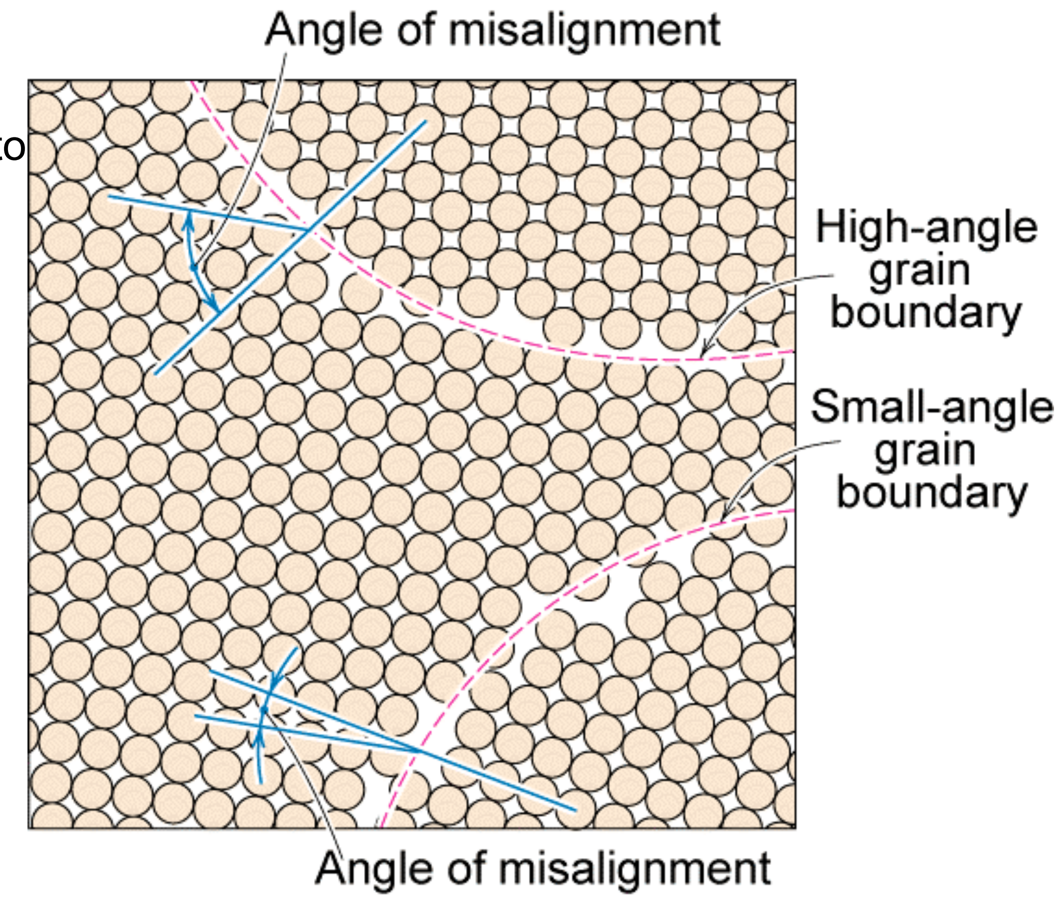
Isotropic

- 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

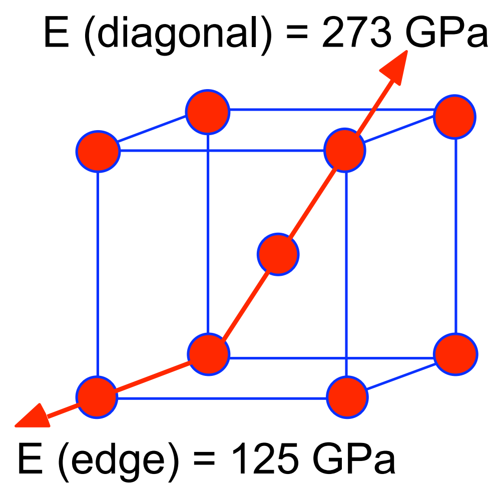
- regions between crystals
- transition from lattice of one region to that of the other
- slightly disordered
- low density in grain boundaries
  - o high mobility
  - o high diffusivity
  - o high chemical reactivity



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

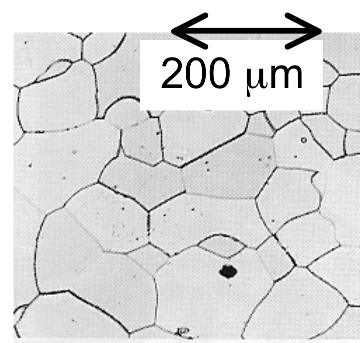
Single crystal vs. Polycrystalline structures

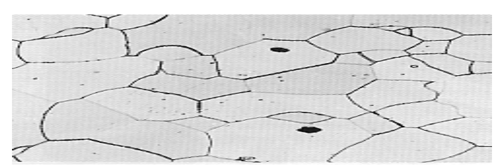
- Single Crystals



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



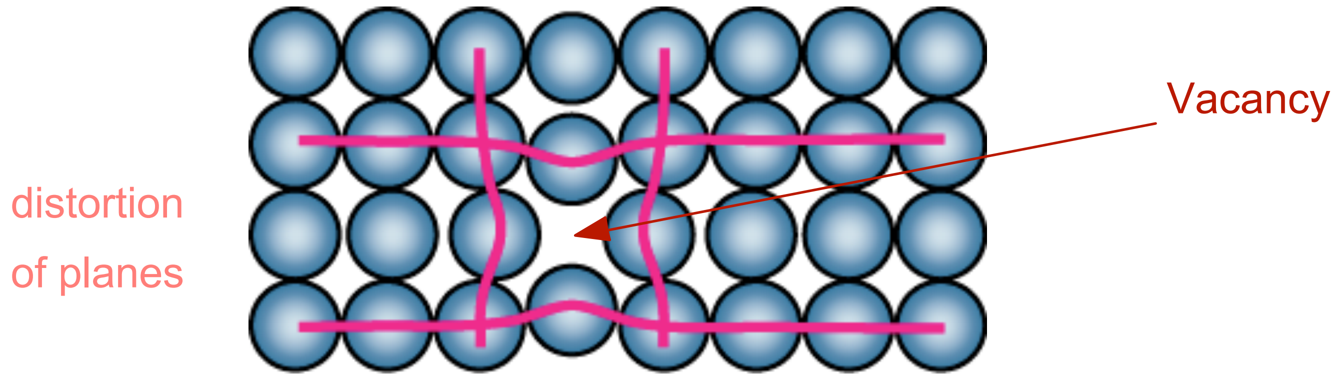


Adapted from Fig. 4.14(b), *Callister 7e*.
(Fig. 4.14(b) is courtesy of L.C. Smith and C. Brady, the National Bureau of Standards, Washington, DC [now the National Institute of Standards and Technology, Gaithersburg, MD].)

Point defects

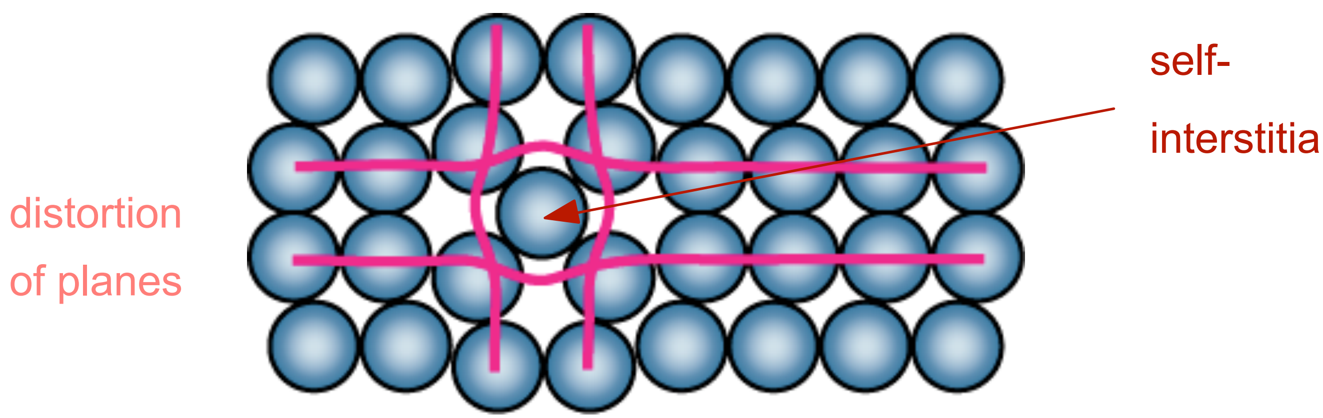
- Vacancies:

  -vacant atomic sites in a structure.



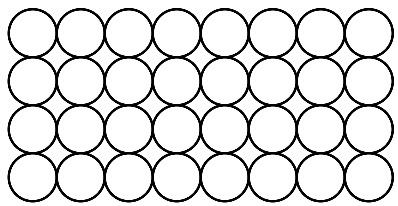
- Self-Interstitials:

  -"extra" atoms positioned between atomic sites.



Equilibrium concentration of defects

- Equilibrium concentration varies with temperature



Each lattice site is a potential vacancy

No. of defects

Activation energy

No. of potential defect sites.

$$\frac{N_v}{N} = \exp\left(\frac{-Q_v}{k\,T}\right)$$

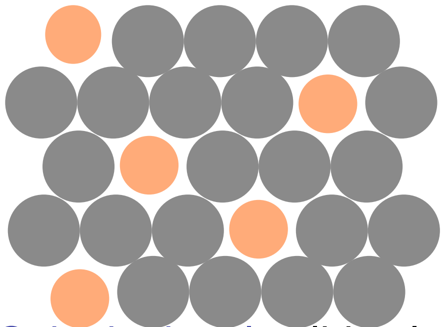
Temperature

Boltzmann's constant

Point defects in alloys

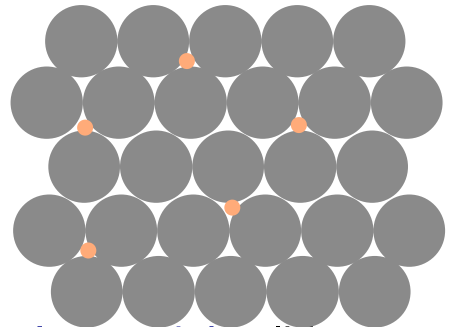
Two outcomes if impurity (B) added to host (A):

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



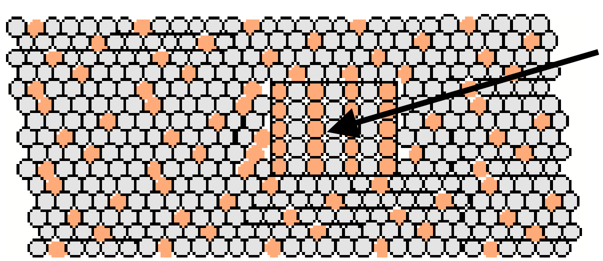
Substitutional solid soln.
(e.g., Cu in Ni)

OR



Interstitial solid soln.
(e.g., C in Fe)

- 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?

Element	*Atomic Radius (nm)*	*Crystal Structure*	*Electro-nega-tivity*	*Valence*
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

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

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
  - **b** $\perp$ to dislocation line
- Screw dislocation:
  - spiral planar ramp resulting from shear deformation
  - **b** $||$ to dislocation line

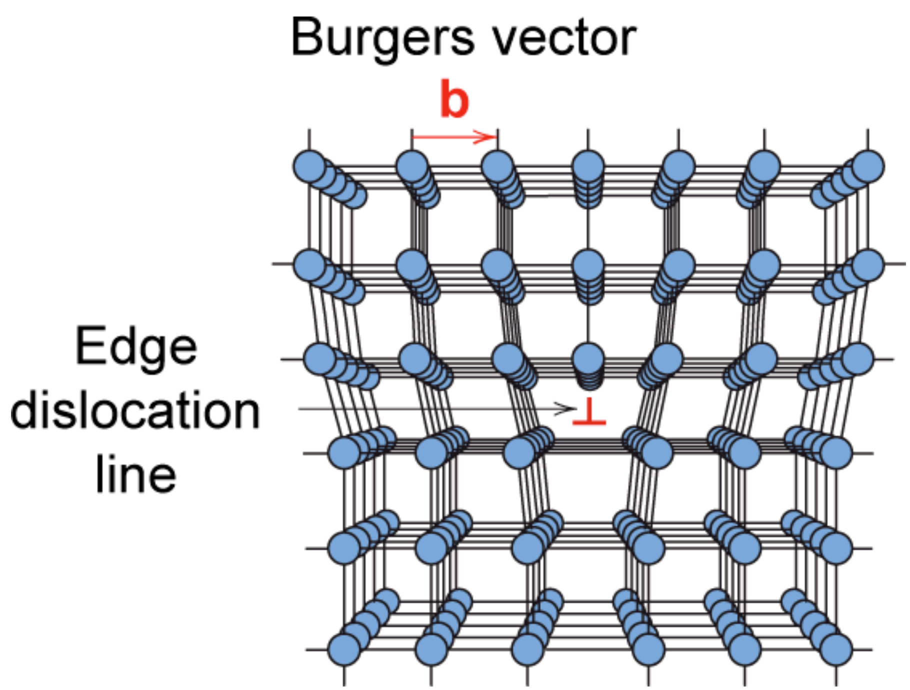
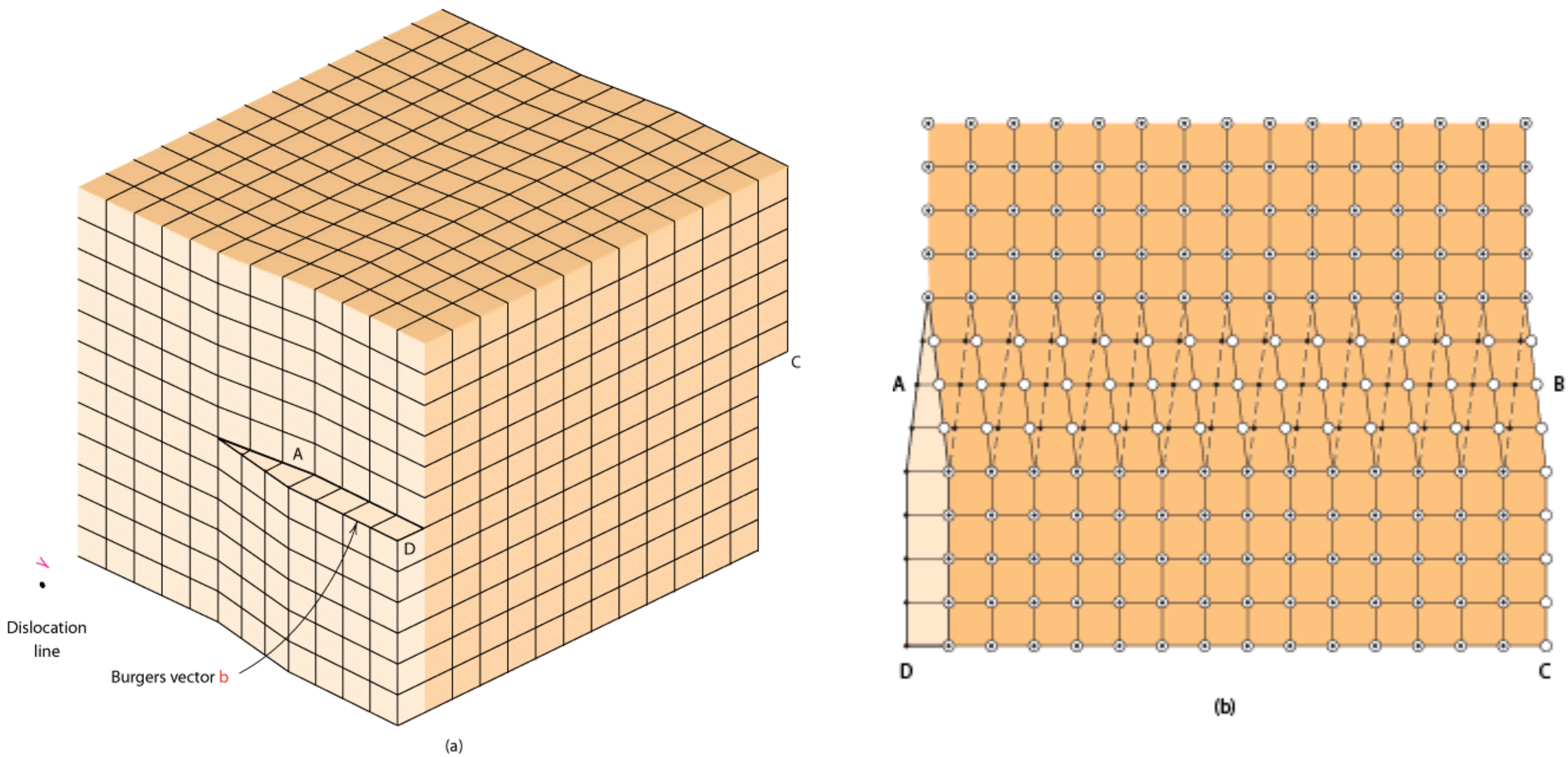


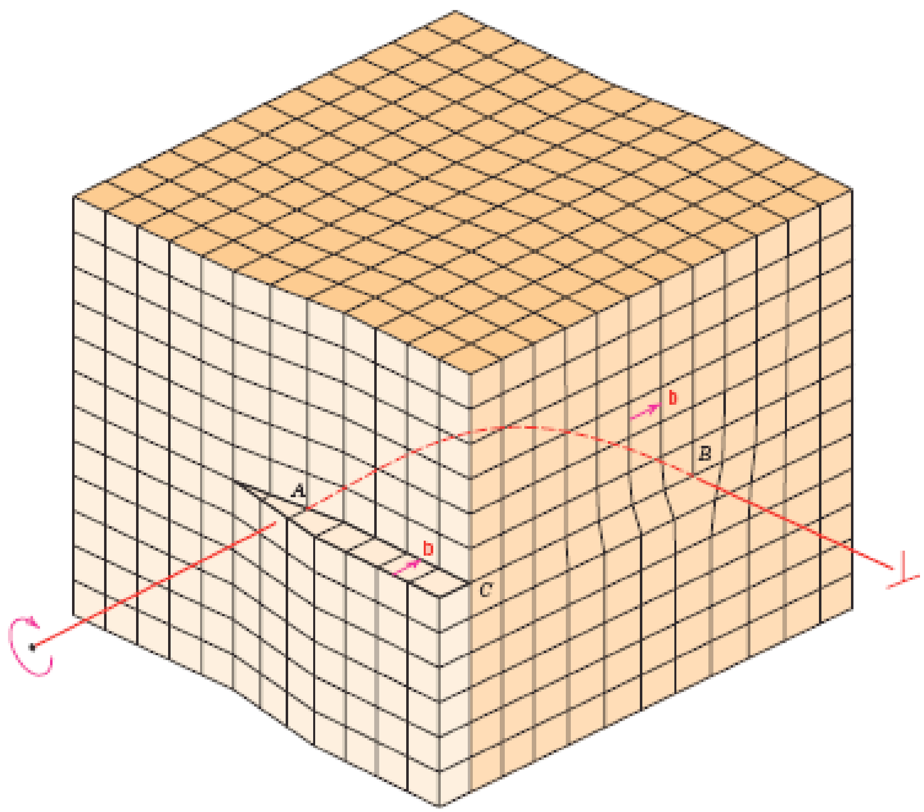
Fig. 4.3, *Callister 7e.*

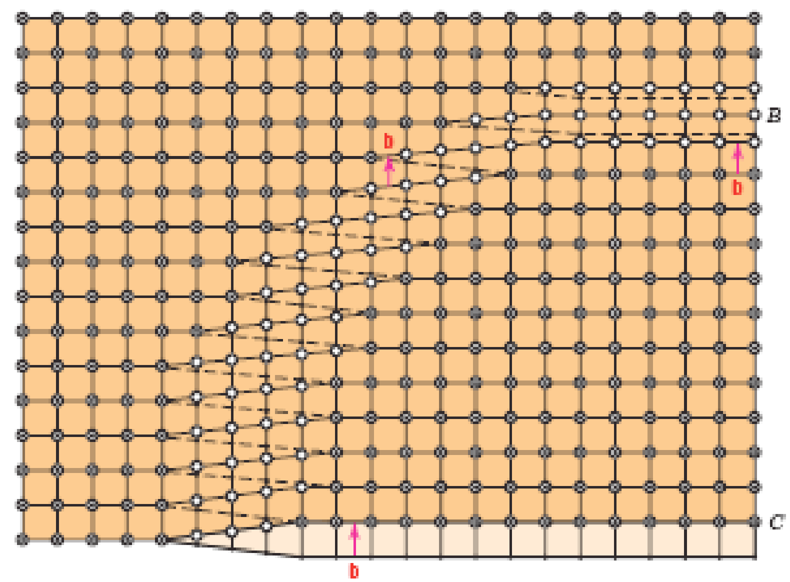
Screw defects



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

Mixed defects

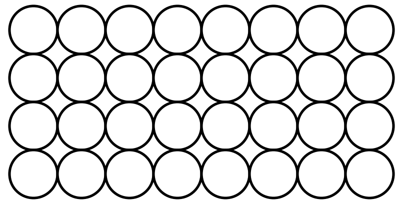




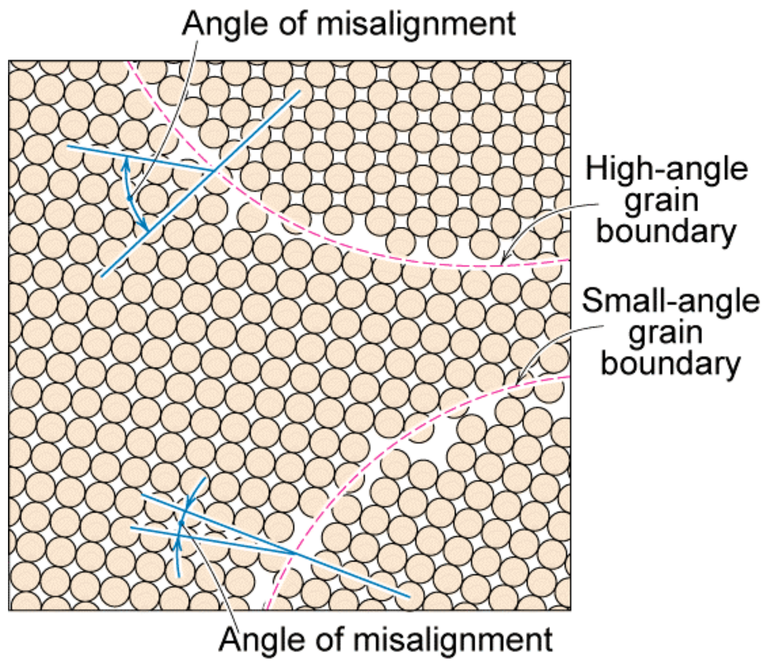
Adapted from Fig. 4.5, *Callister 7e.*

Planar defects

- External defects
  - On the surface
  - Unsatisfied bonds

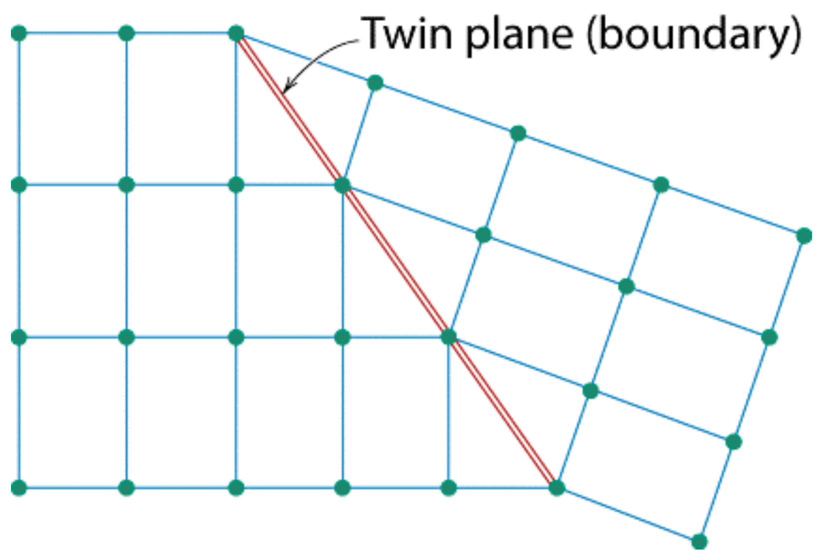


- Internal defects
  - Grain boundaries



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