Chemical Engineering 378

Science of Materials Engineering

Lecture 5

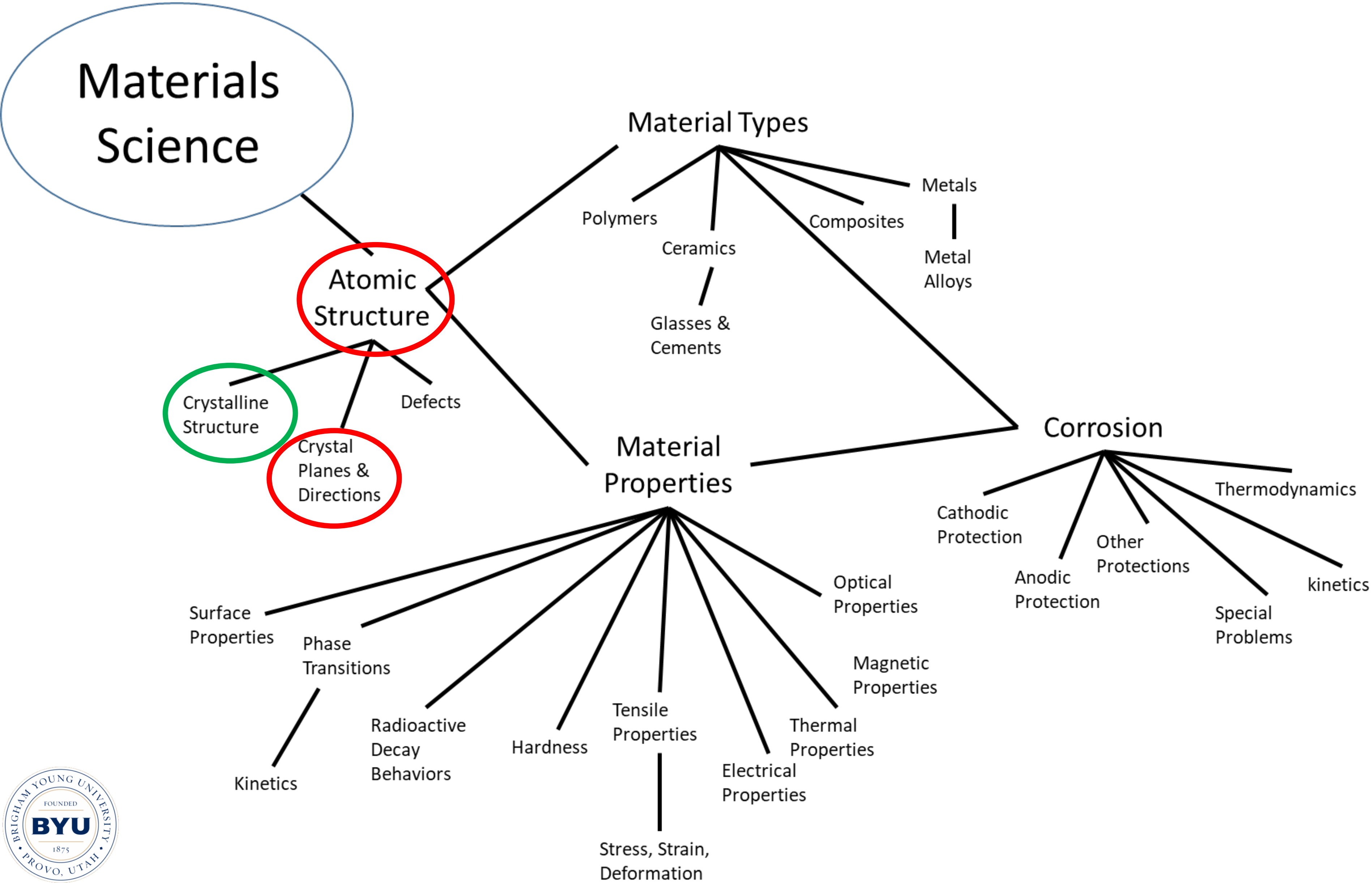
Planar/Linear Density & Crystallinity

Spiritual Thought

We have all been injured or wronged by someone else. We didn’t deserve it. Some of us have lost a loved one prematurely through the negligence or recklessness of another. That is so unfair and cannot be undone by monetizing our pain in court. Moreover, in the simple process of living, we are likely to experience crippling pains and injuries, debilitating conditions, and undeserved infirmities of mind and body. All these persist forever if there be no Christ.

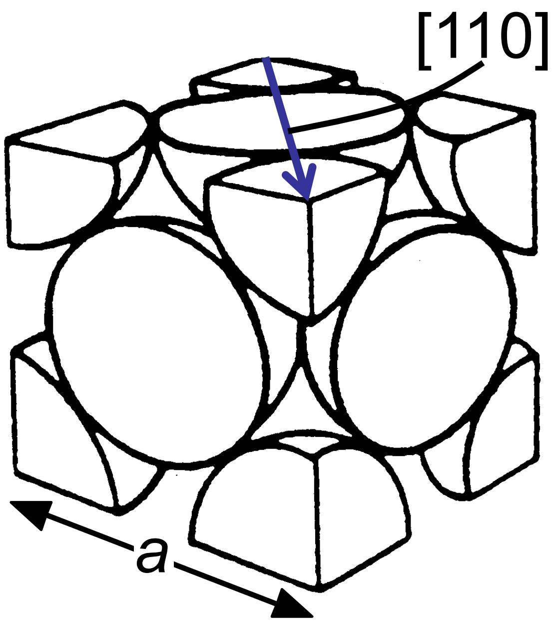
-Elder Kyle McKay

Materials Roadmap



Linear Density

- Linear Density of Atoms $\equiv$ LD = $\dfrac{\text{Number of atoms}}{\text{Length of direction vector}}$



Adapted from Fig. 3.1(a), *Callister & Rethwisch 8e.*

ex: linear density of Al in [110] direction

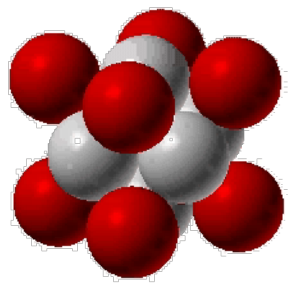
a = 0.405 nm

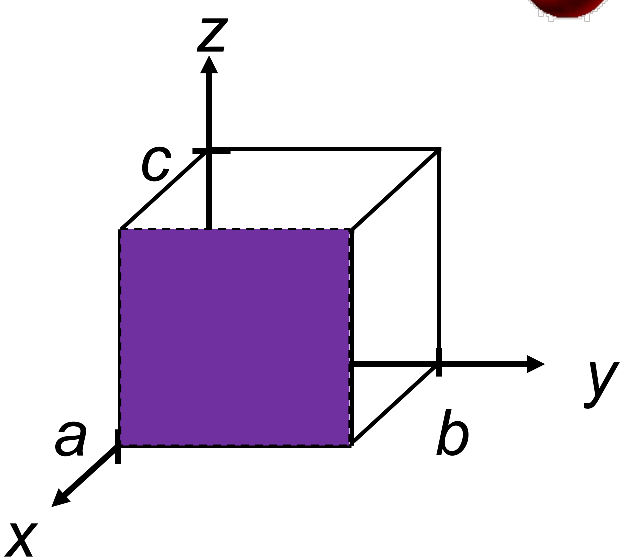
atoms

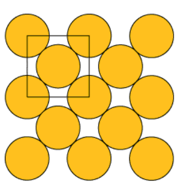
length

$$LD = \frac{2}{\sqrt{2}a} = \boxed{3.5\ \text{nm}^{-1}}$$

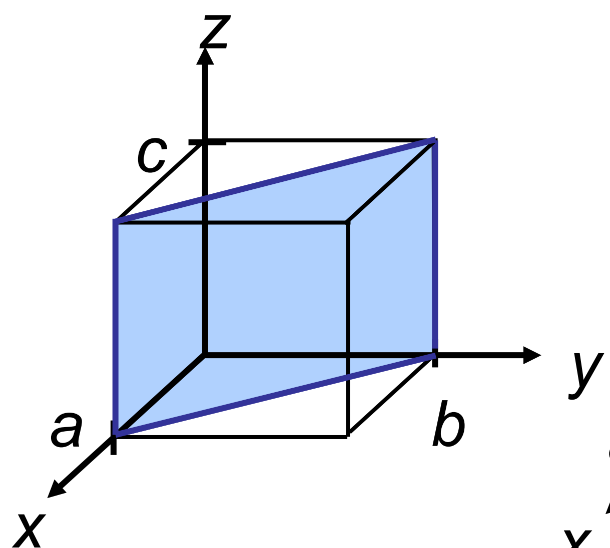
Look at FCC Planes

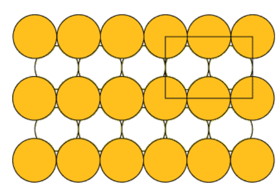




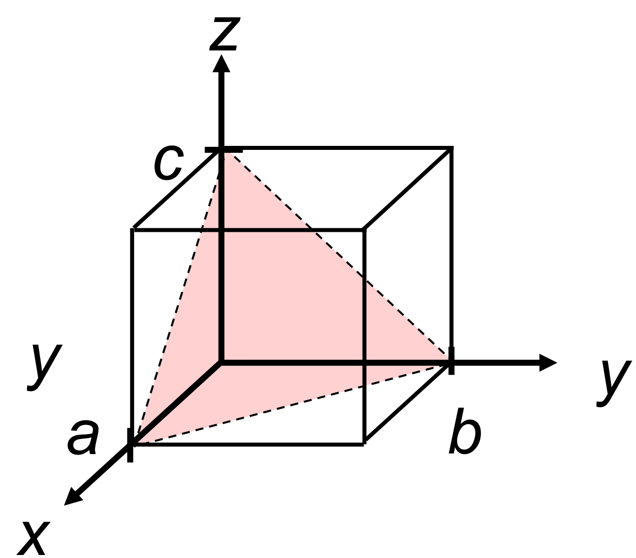


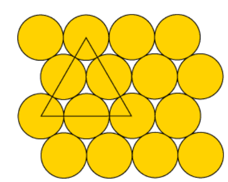
(100)





(110)





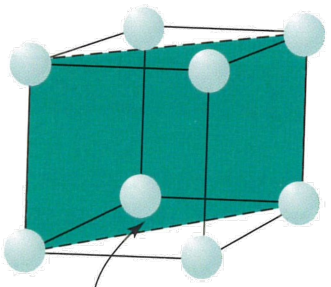
(111)

Planar Density – SC Cell

- What is the area of the (110) plane in terms of the lattice parameter?
- What is the area of the (110) plane in terms of the atomic radius?
- What is the total area of atoms that lie on the (110) plane?

- The planar density is defined as
  PD= # atoms with their center in the plane /
  Area of plane (i.e. 2D repeat unit)

- Concept Check
  - What is the PD for (110) in a SC unit cell?



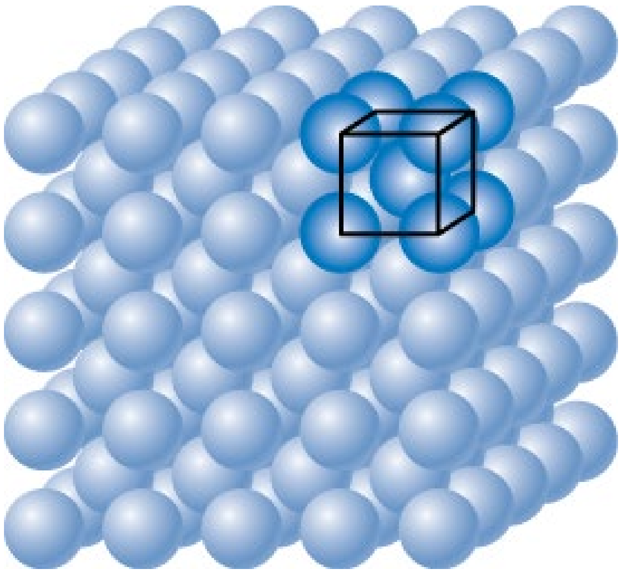
Guided Inquiries from “Introduction to Materials Science and Engineering: A Guided Inquiry” by Elliot P. Douglas, Pearson Higher Education, 2014.

Crystallographic Planes

- We want to examine the atomic packing of crystallographic planes.
- Why? Iron foil can be used as a catalyst for carbon nanotubes.
- 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.

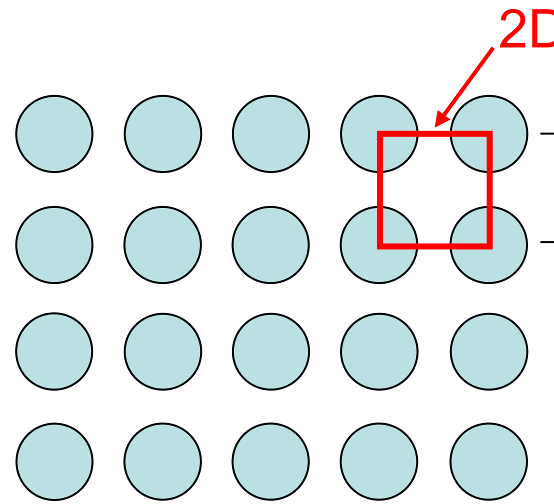
Planar Density of (100) Iron

Solution: At T < 912ºC iron has the BCC structure.



Adapted from Fig. 3.2(c), *Callister & Rethwisch 8e.*

(100)



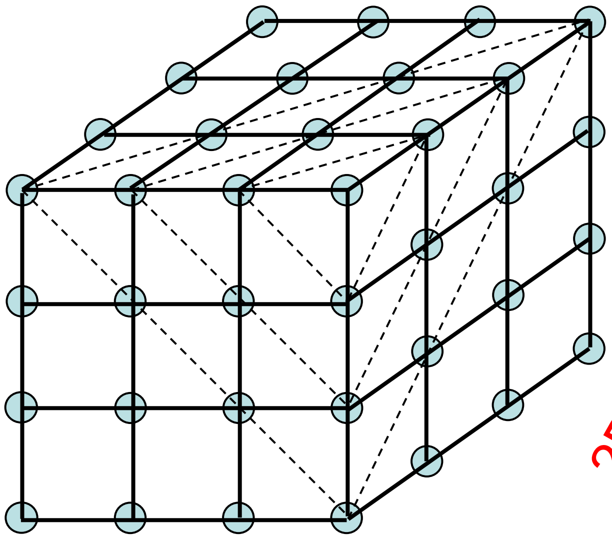
$$a = \frac{4\sqrt{3}}{3}R$$

Radius of iron R = 0.1241 nm

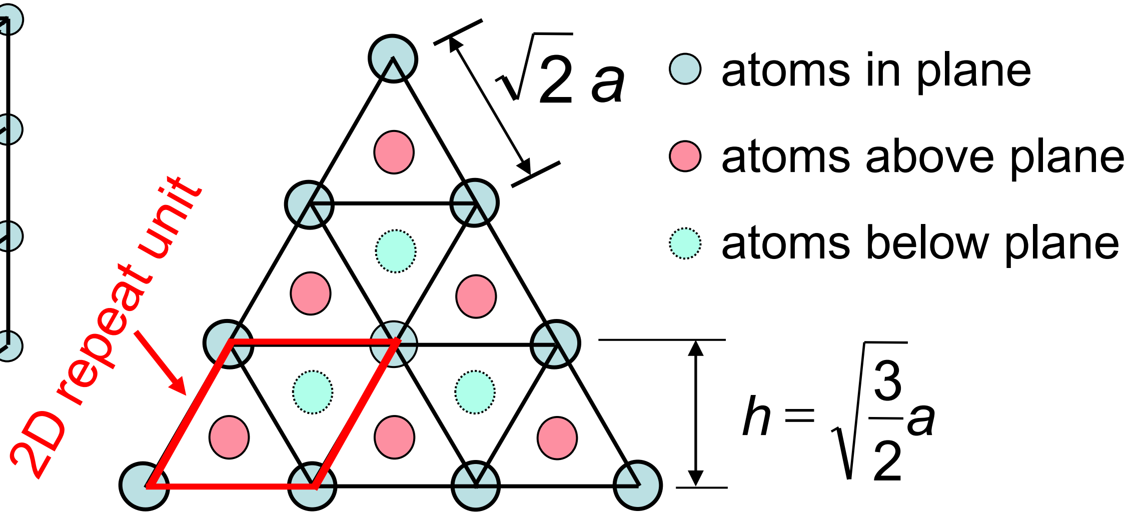
$$\text{Planar Density} = \frac{\overset{\text{atoms / 2D repeat unit}}{1}}{\underset{\text{area / 2D repeat unit}}{a^2}} = \frac{1}{\left(\frac{4\sqrt{3}}{3}R\right)^2} = 12.1\,\frac{\text{atoms}}{\text{nm}^2} = \boxed{1.2 \times 10^{19}\,\frac{\text{atoms}}{\text{m}^2}}$$

Planar Density of (111) Iron

Solution (cont): (111) plane

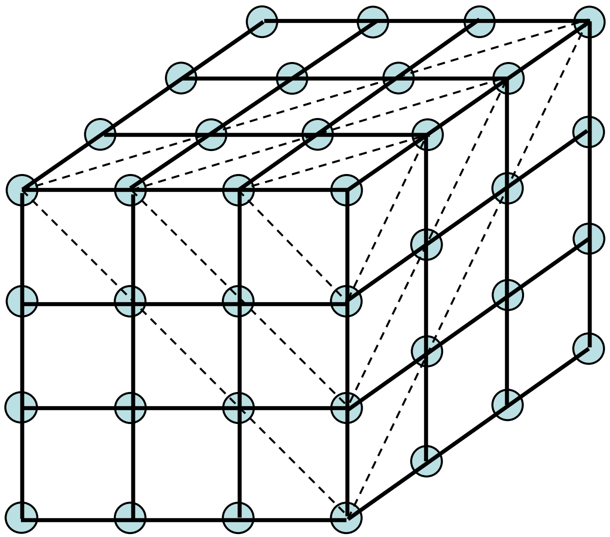


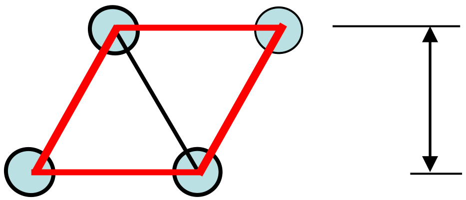
1 atom in plane/ unit surface cell



Planar Density of (111) Iron

Solution (cont): (111) plane





$$h = \sqrt{\frac{3}{2}}a$$

$$\text{area} = \sqrt{2}\,ah = \sqrt{3}\,a^2 = \sqrt{3}\left(\frac{4\sqrt{3}}{3}R\right)^2 = \frac{16\sqrt{3}}{3}R^2$$

$$\frac{\text{atoms}}{\text{2D repeat unit}}$$

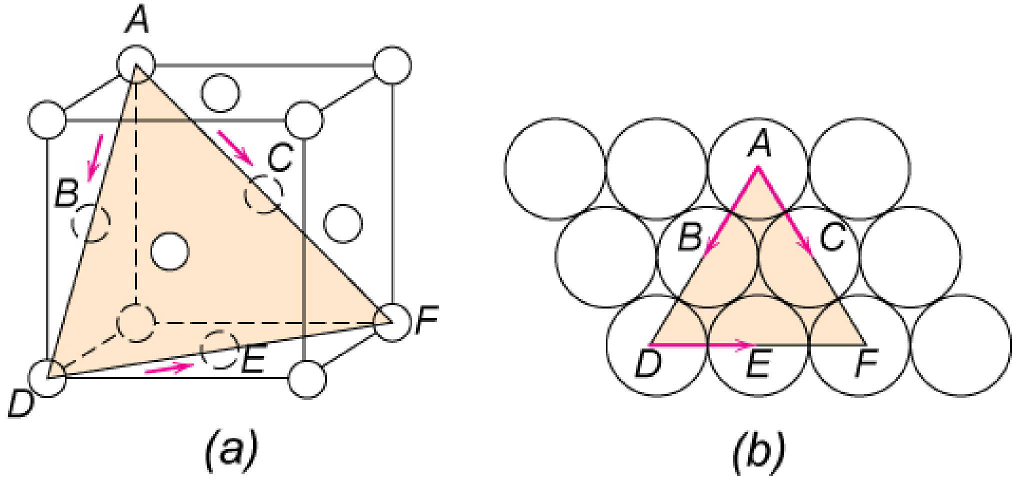
$$\text{Planar Density} = \frac{1}{\frac{16\sqrt{3}}{3}R^2} = 7.0\,\frac{\text{atoms}}{\text{nm}^2} = \boxed{0.70 \times 10^{19}\,\frac{\text{atoms}}{\text{m}^2}}$$

$$\frac{\text{area}}{\text{2D repeat unit}}$$

Ch 7 preview

Slip System

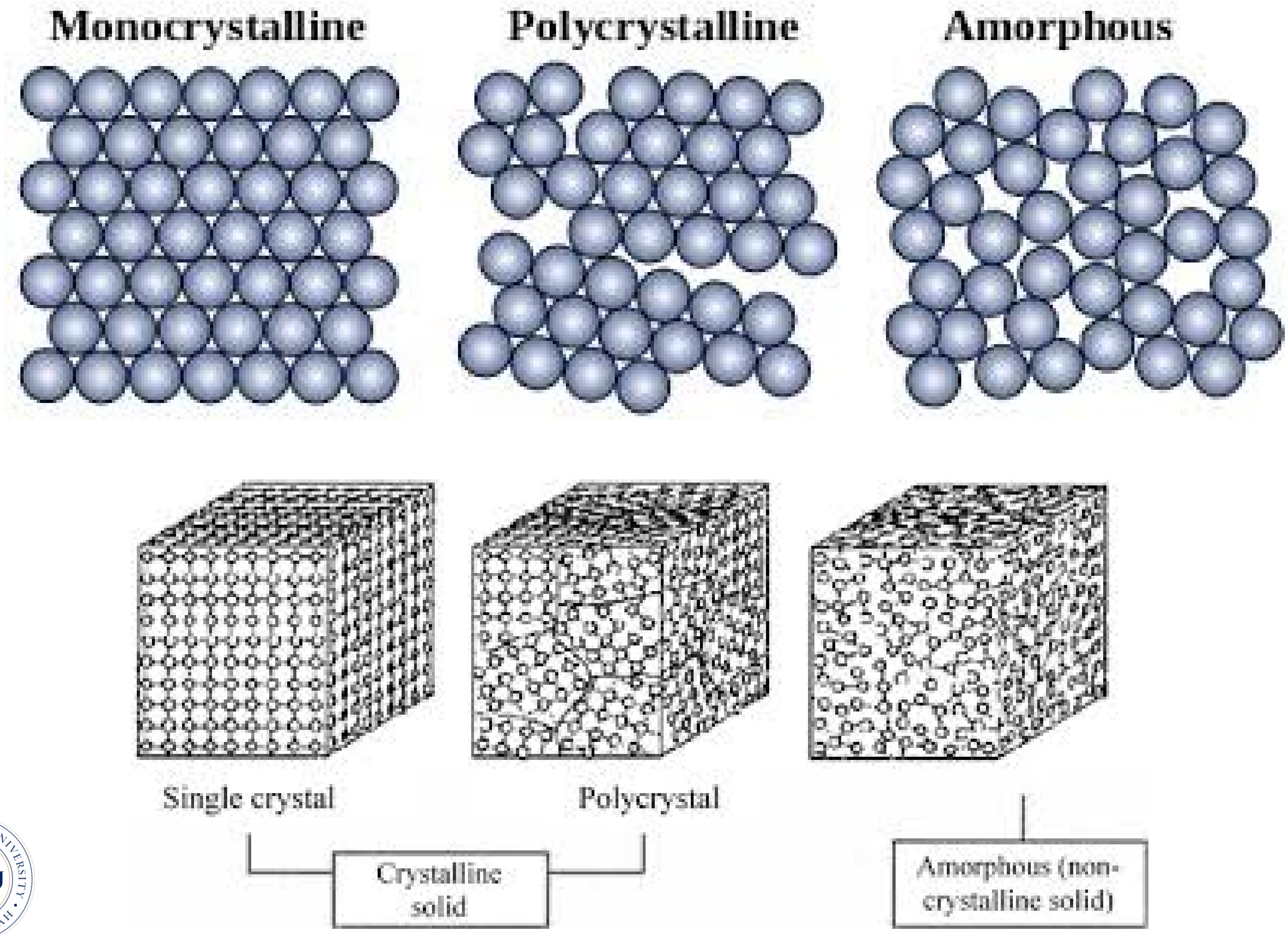
- Slip plane - plane on which easiest slippage occurs
  - Highest planar densities (and large interplanar spacings)
- Slip directions - directions of movement
  - Highest linear densities



Adapted from Fig. 7.6, *Callister & Rethwisch 8e.*

- FCC Slip occurs on {111} planes (close-packed) in <110> directions (close-packed)

Reality of Materials



Crystals as Building Blocks

- *Some* engineering applications require single crystals:

  -- diamond single crystals for abrasives

(Courtesy Martin Deakins, GE Superabrasives, Worthington, OH. Used with permission.)

  -- turbine blades

Fig. 8.33(c), *Callister & Rethwisch 8e.* (Fig. 8.33(c) courtesy of Pratt and Whitney).

- Properties of crystalline materials often related to crystal structure.

  -- Ex: Quartz fractures more easily along some crystal planes than others.

  -- Ex: Silicon wafers snap really cleanly along some planes (100)

(Courtesy P.M. Anderson)

Polycrystals

Anisotropic

- *Most* engineering materials are polycrystals.

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

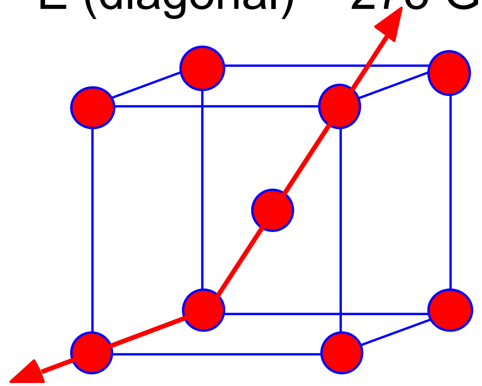
Isotropic

- 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 typically range from 1 nm to 2 cm
  (i.e., from a few to millions of atomic layers).

Single vs Polycrystals

- Single Crystals
  - -Properties vary with direction: anisotropic.
  - -Example: the modulus of elasticity (E) in BCC iron:

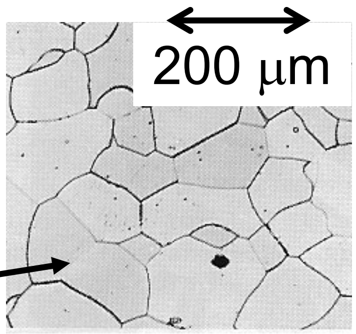
E (diagonal) = 273 GPa

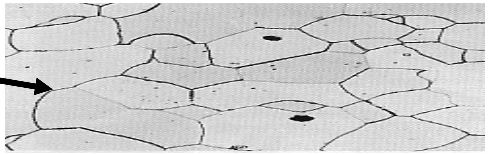


E (edge) = 125 GPa

Data from Table 3.3, *Callister & Rethwisch 8e*. (Source of data is R.W. Hertzberg, *Deformation and Fracture Mechanics of Engineering Materials*, 3rd ed., John Wiley and Sons, 1989.)

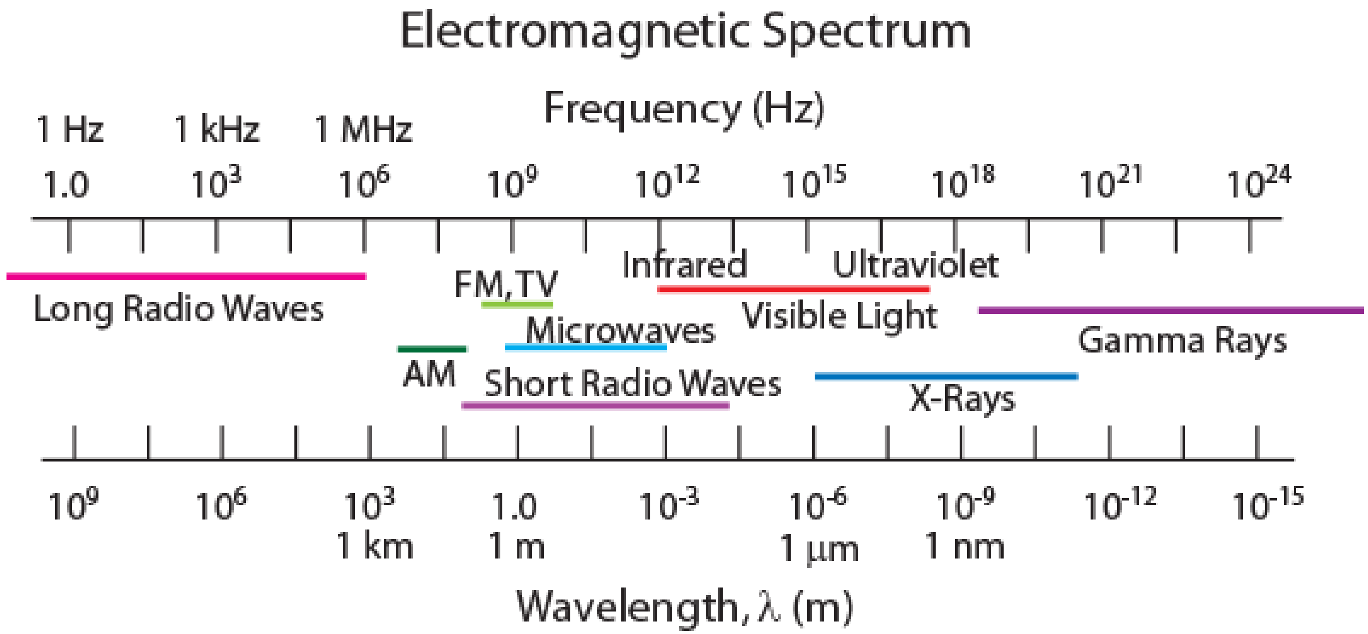
- Polycrystals
  - -Properties may/may not vary with direction.
  - -If grains are randomly oriented: isotropic. ($E_{poly\ iron}$ = 210 GPa)
  - -If grains are textured, anisotropic.





Adapted from Fig. 4.14(b), *Callister & Rethwisch 8e*. (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].)

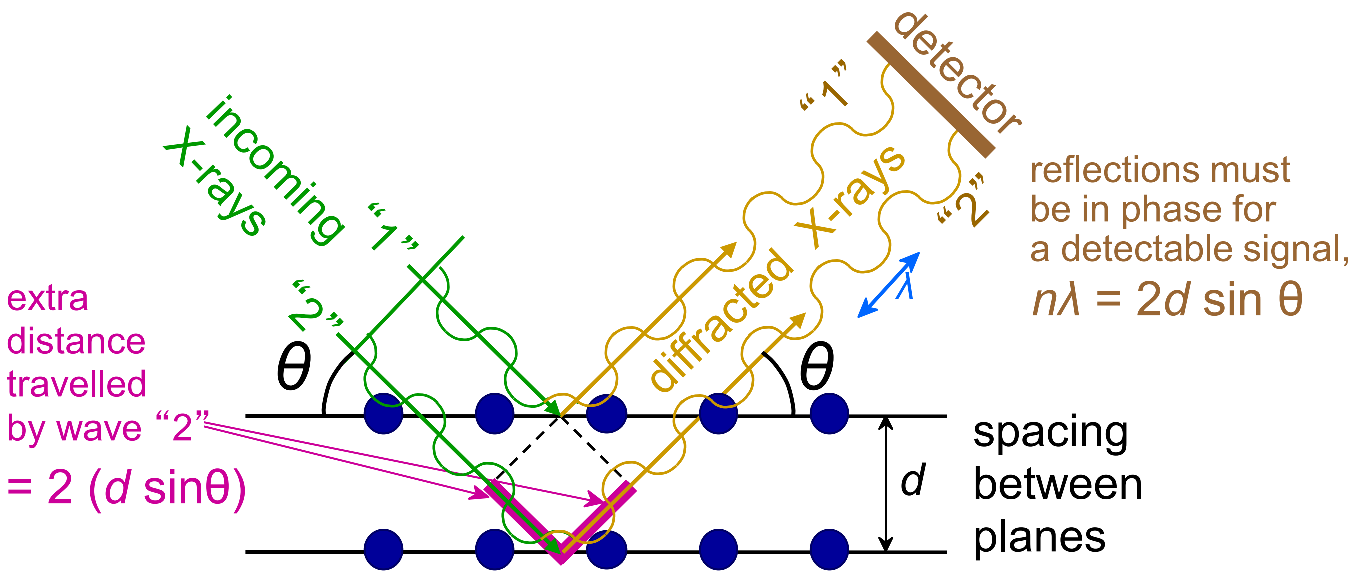
X-Ray Diffraction



- Diffraction gratings must have spacings comparable to the wavelength of diffracted radiation.
- Can't resolve spacings $< \lambda$
- Spacing is the distance between parallel planes of atoms.

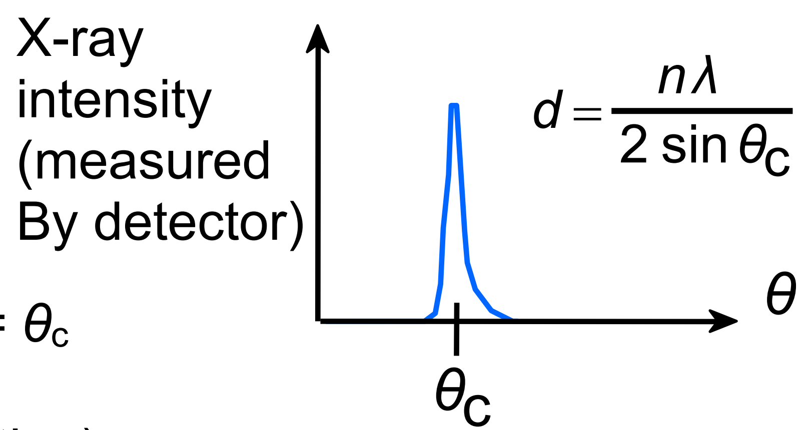
X-Rays to Determine Crystal Structure

- Crystallographic planes diffract incoming X-rays



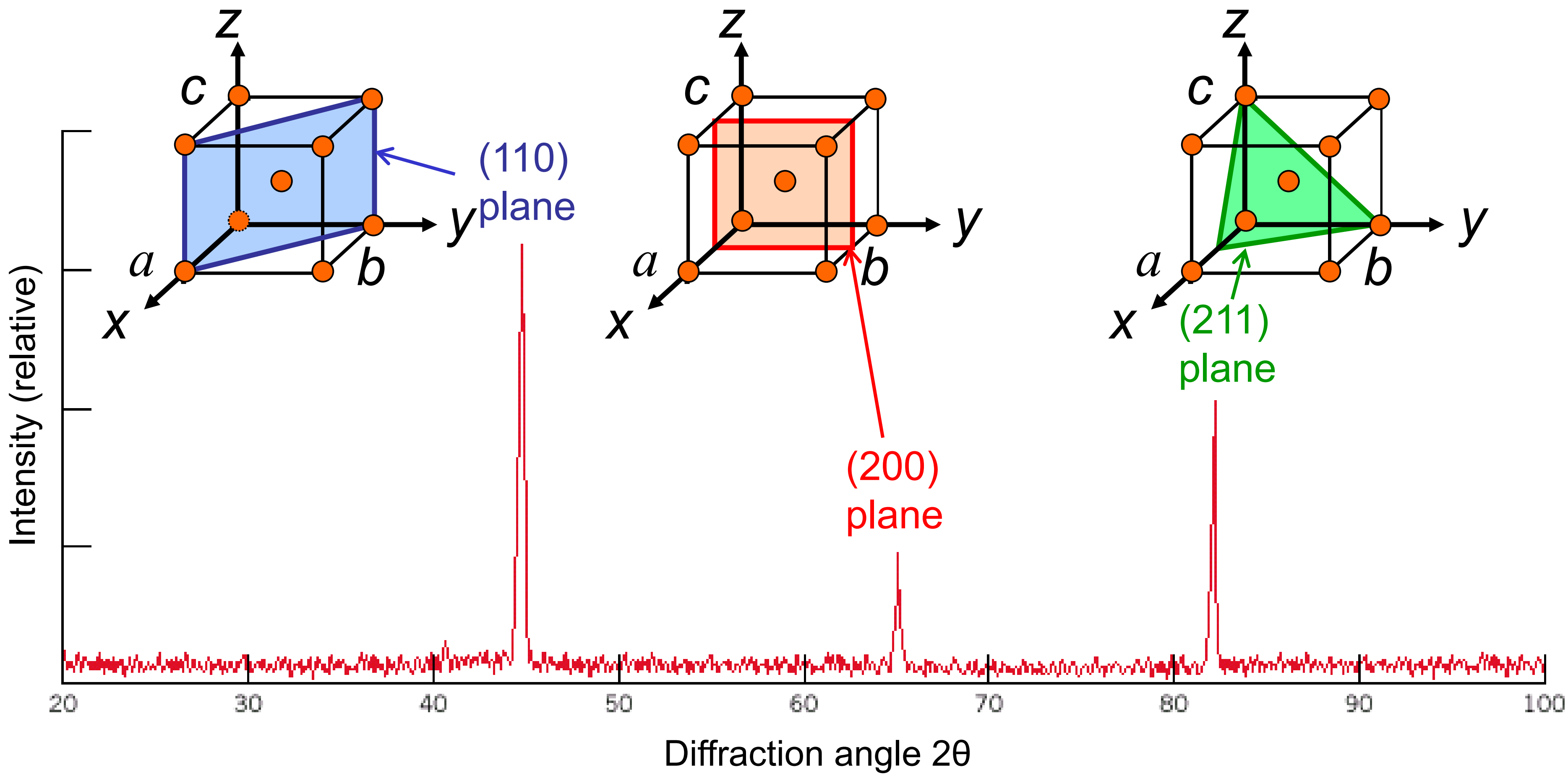
Measurement of diffraction angle, θ_c, allows computation of interplanar spacing, d.

Diffraction occurs when $\theta = \theta_c$



(n = the order of reflection)

X-Ray Diffraction Pattern



Diffraction pattern for polycrystalline α-iron (BCC)