Outline (Chapter 3)

- **Atomic Packing:**
  - ✓Linear density
  - ✓Planer density
- **Single-crystal & Polycrystalline Materials**
- **Crystal Structure Analysis: *X-ray Diffraction***

Atomic Packing

➢ **Arrangement of atoms on different directions and in different planes are called linear and planar densities, respectively.**

✓ **Importance:**

- Deformation in metals **(Slip)** depends on linear & planar density (WHY?):
- Because slip occurs on planes that have the greatest density of atoms in direction with highest density ***(along closest packed directions on the closest packed planes)***

Atomic Packing

- **Linear Density**

Number of atoms/length whose centers lie on the direction vector for a specific crystallographic direction. **(# of atoms/unit length)**

$$\text{Linear Density of Atoms} \equiv \text{LD} = \frac{\text{Number of atoms}}{\text{Unit length of direction vector}}$$

- **Planar Density**

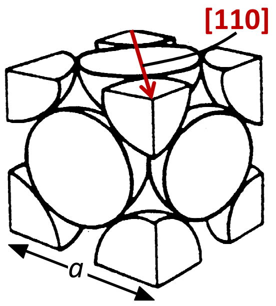
Number of atoms/unit area that are centered on a particular crystallographic plane. **(# of atoms/unit area)**

$$\text{Planar Density of Atoms} \equiv \text{PD} = \frac{\text{Number of atoms}}{\text{Area of the plane}}$$

Linear Density

- **Example:**

linear density of Al in [110] direction , a = 0.405 nm



atoms

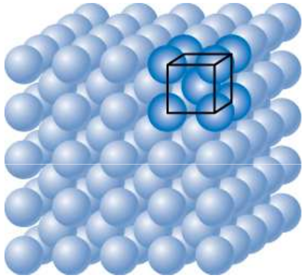
$$\text{LD} = \frac{2}{\sqrt{2}a} = \boxed{3.5 \text{ atoms/nm}}$$

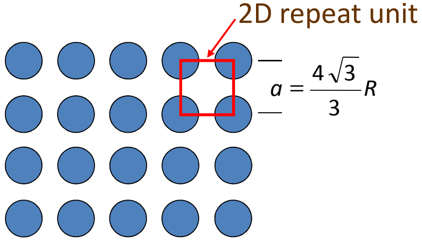
length

Planar Density

- **Example:** Planar density of iron (at T < 912°C) in **(100)** plane.

At T < 912°C Iron has BCC crystal structure





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

Radius of iron R = 0.1241 nm

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

Planar Density

- **FCC** and **HCP** are both **CLOSE-PACKED** structures.

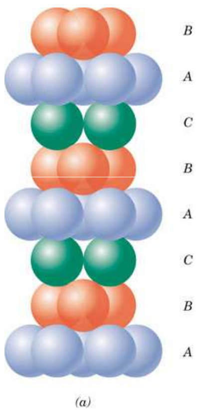
APF = 0.74: This is the maximum if all atoms are same size.

- Atoms are packed in CLOSE-PACKED planes:
  (*but different stacking sequence*)
  - ✓ In **FCC, {111}** are close packed planes (stack as **ABC-ABC-ABC**)
  - ✓ In **HCP, (0001)** is close packed plane (stack as **AB-AB-AB-AB**)

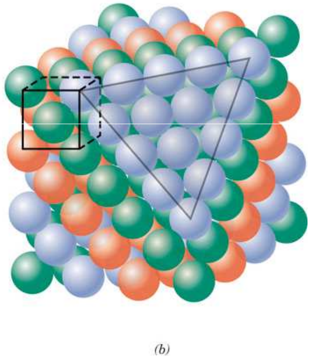
➢ **Note:** *BCC is not close packed (APF = 0.68), the most densely packed plane is {110}*

Planar Density

FCC



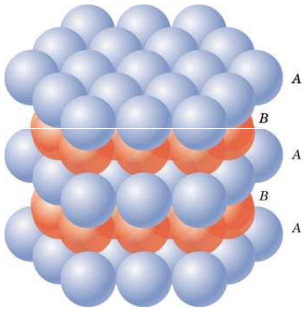
(a)



(b)

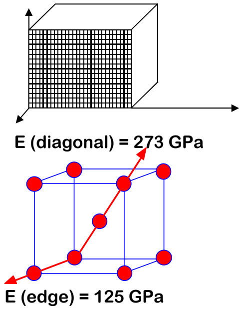
(111)

HCP



(0001)

Single-Crystal vs. Polycrystalline



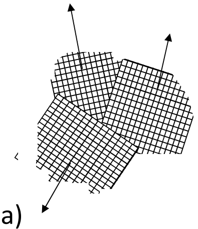
SINGLE CRYSTALS

✓ This is when a piece of material is made up of one crystal;

✓ All the unit cells are aligned up in the same orientation

✓ Properties vary with direction **(anisotropic)**.

e.g. Stiffness (rigidity) electrical conductivity, refraction.



POLYCRYSTAL

✓ Many small **crystals (grains)** with **different orientations** joined together. (each grain is a single crystal)

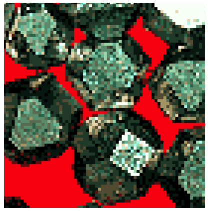
✓ Most engineering materials are POLYCRYSTALLINE.

✓ **Grain boundary:** Regions where grains (crystals) meet.

✓ If crystals are **randomly** oriented, overall component properties are not directional **(isotropic).** ($E_{\text{poly iron}}$ = 210 GPa)

Single-Crystals

- Some engineering applications require single crystals:



-- diamond single crystals for abrasives

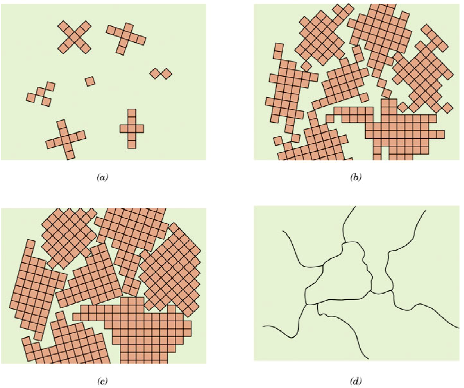
--turbine blades

-- Crystal properties reveal features of atomic structure.

--Ex: Certain crystal planes in quartz fracture more easily than others.

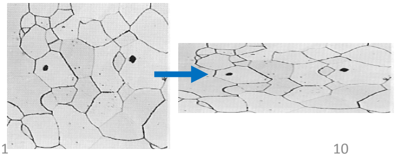
Polycrystalline Materials

- Solidification of a polycrystalline material



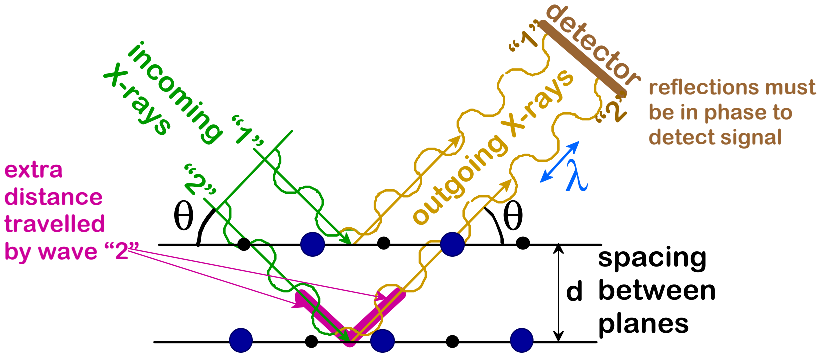
✓ If crystals are **randomly** oriented, overall component properties are not directional **(isotropic).**

✓ If grains are **textured** (e.g., after rolling), **anisotropic.**



Crystal Structure Analysis: *X-ray Diffraction*

- **Incoming X-rays diffract from crystal planes.**



- **Measurement of: Critical angles, θ_c, for X-rays provide atomic spacing, d_{hkl}.**

Crystal Structure Analysis: *X-ray Diffraction*

- **Finding out What the Crystal Structure is.**

Analysis using X-Rays. X-Ray Diffraction.

- **Bragg's Law:**

  ✓ Incoming X-rays diffract from crystal planes.

  ✓ X-rays are diffracted off atoms and either constructively interfere (peak) or destructively interfere (low) from layers of atoms depending on interplanar spacing (d_{hkl}) and angle.

$$\boxed{n\lambda = 2d_{hkl}\sin\theta} \qquad \text{(Bragg's Law)}$$

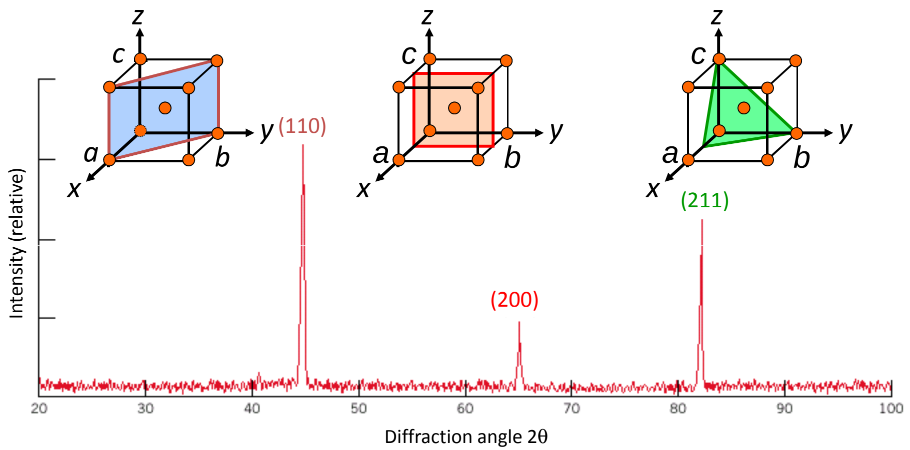
n = 1,2, 3, 4, 5.......
λ = wavelength of incident X-rays
θ = incident angle

Crystal Structure Analysis: *X-ray Diffraction*

- As θ is varied, peaks will occur when distance SQT is a whole number of wavelengths.
- So can measure peak and use Bragg's law to determine d_{hkl} and then "a".
- Distance between similar planes in the cubic systems, e.g., (110) planes in adjacent unit cells:

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

X-ray Diffraction



Diffraction pattern for polycrystalline α-iron (BCC)

X-ray Diffraction (review problem)

- **For BCC Fe, compute:**

(a) the interplanar spacing and,
(b) the diffraction angle for (220) set of planes.

– The lattice parameter for Fe is 0.2866 nm
– the wavelength used is 0.1790 nm
– First order reflection.

Summary

- **Atoms may assemble into crystalline or amorphous structures.**
- **We can predict the density of a material, provided we know the atomic weight, atomic radius, and crystal geometry (e.g., FCC, BCC, HCP).**
- **Material properties generally vary with single crystal orientation (i.e., they are anisotropic), but properties are generally non-directional (i.e., they are isotropic) in polycrystals with randomly oriented grains.**