Outline:

- Atomic Densities
    - Linear Density
    - Planar Density
- Single- vs poly- crystalline materials
- X-ray Diffraction
- Example
- Polymorphism and Allotropy

Atomic Densities

- **Linear Density**

– Number of atoms per length whose centers lie on the direction vector for a specific crystallographic direction.

$$\text{Linear Density} = \frac{\text{Number of atoms centered on direction vector}}{\text{length of direction vector}}$$

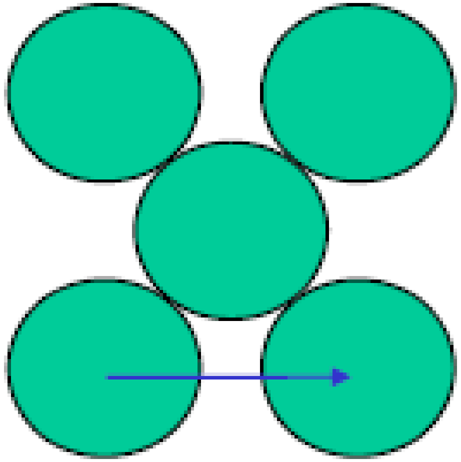
- **Planar Density**

– Number of atoms per unit area that are centered on a particular crystallographic plane.

$$\text{Planar Density} = \frac{\text{Number of atoms centered on a plane}}{\text{area of the plane}}$$

Linear Density

- Calculate the linear density of the [100] direction for the FCC crystal



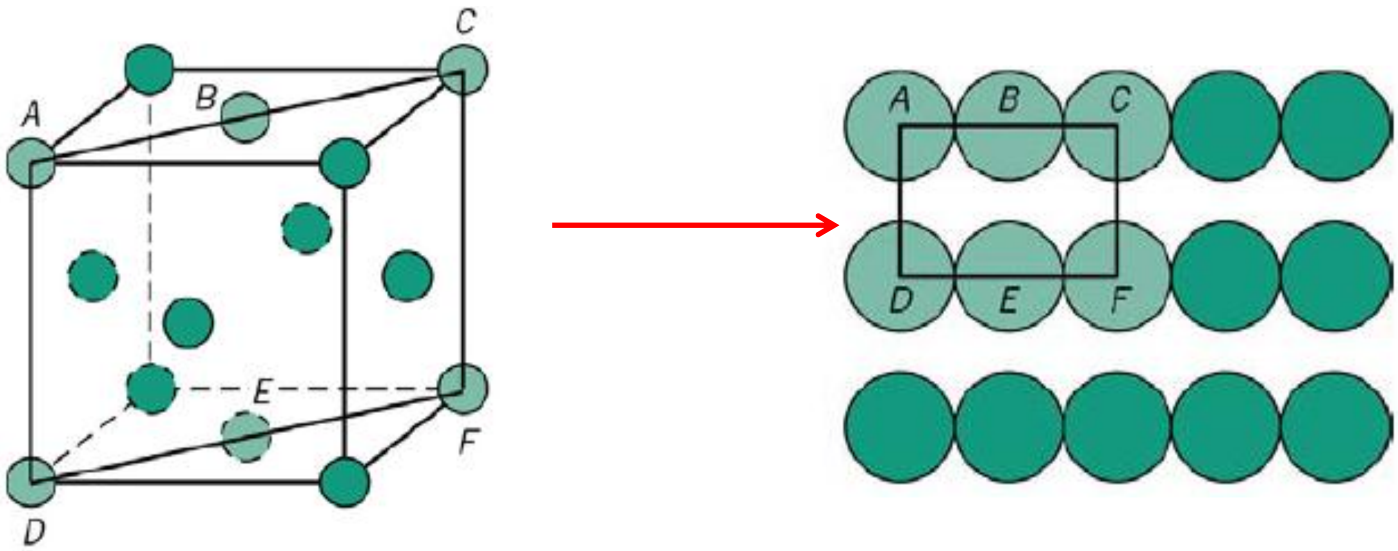
$LD = n/L_L$ linear density

$n = 0.5$ atoms

L_L= a line length

Planar Density

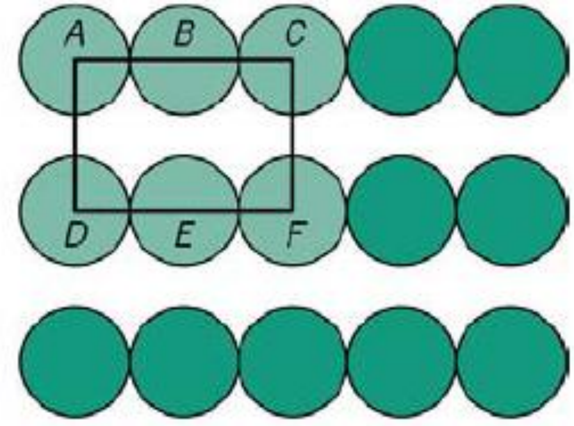
- Calculate the planer density of the (110) plane for the FCC crystal



- Compute planar area
- Compute number of atoms

For an atom to be counted, it has to be centered on that plane.

Planar Density



Plane area $A_P = (AC)\times(AD)$

AC =…**4 R**……

AD = …**a**…. $where\ a = 2\sqrt{2}R$

Area = …$8\sqrt{2}R^2$…

Number of atoms = **2 atoms**

$$PD = \frac{n}{A_P} = \frac{2}{8\sqrt{2}R^2}$$

Linear and Planar Density

- Why do we care?
- Properties, in general, depend on linear and planar density.

• Examples:

✓ Speed of sound along directions
✓ Slip (deformation in metals) depends on linear and planar density
✓ Slip occurs on planes that have the greatest density of atoms in direction with highest density

we would say along closest packed directions on the closest packed planes

Crystals As Building Blocks

- *Some* engineering applications require single crystals:

Single crystal

(Courtesy P.M. Anderson)

- Turbine blades
- Nickel alloy – single crystal
- to improve high temp. mechanical properties

Fig. 8.30(c), *Callister 6e.*
(courtesy of Pratt and Whitney)

(Courtesy GE Superabrasives)

- diamond single crystals for abrasives

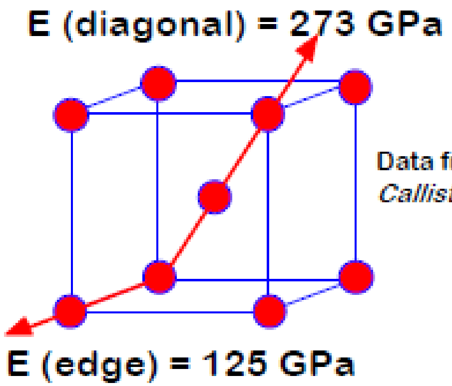
- *Most* engineering materials are polycrystals.

✓ Each "grain" is a single crystal.
✓ If crystals are randomly oriented, overall component properties are not directional.
✓ Crystal sizes typ. range from 1 nm to 2 cm
(i.e., *from a few to millions of atomic layers*).

Nb-Hf-W plate with an electron beam weld

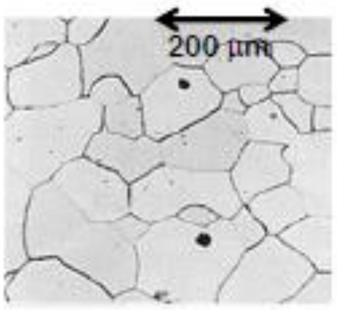
Single Vs Polycrystals

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

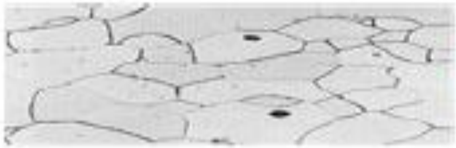


Data from Table 3.3, *Callister 6e.*

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



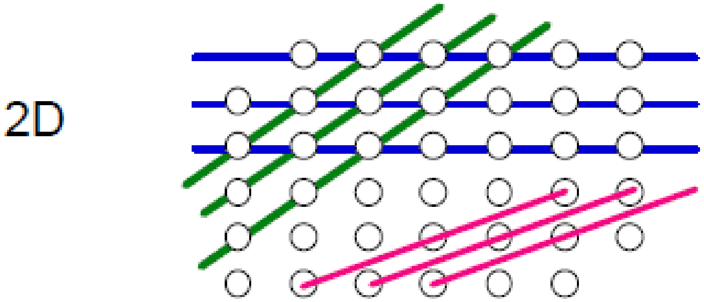
Adapted from Fig. 4.12(b), *Callister 6e.*



Textured grains

Polycrystalline materials, crystallographic orientations of the individual grains are totally random. Even though each grain may be anisotropic. A specimen composed of grains behave isotropically.

Inter-Planar Spacing & X-Ray Diffraction



- Inter-planar spacing

– *The inter-planar spacing in a particular direction is the distance between equivalent planes of atoms*

- The existence of, and distances between sets of planes in a material is characteristic for each material

- Inter-planar spacings are measured by x-ray diffraction to identify unknown materials!

X-Ray Diffraction

- Can be used to determine crystal structure
  - identify unknown materials
  - measure lattice parameters

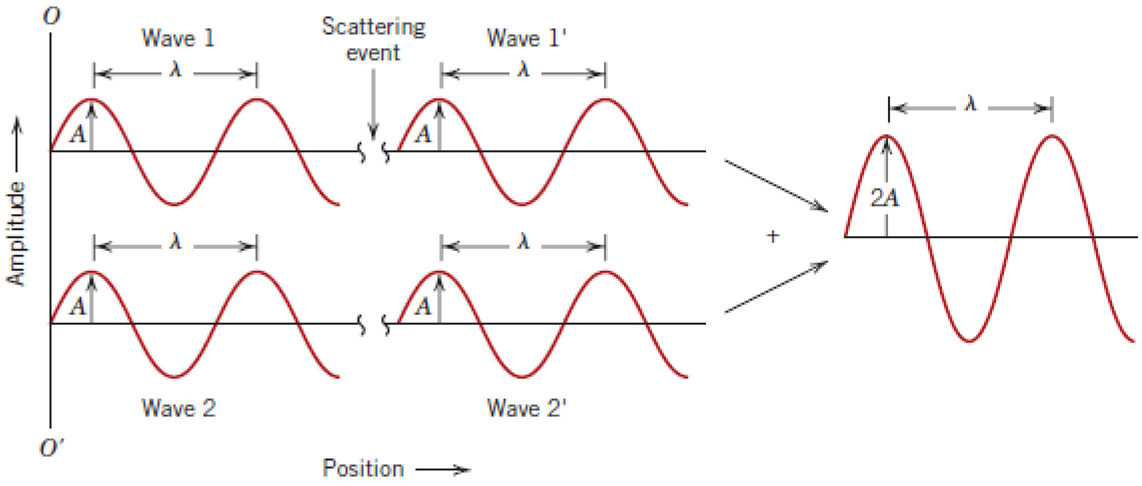
- X-rays are a form of electromagnetic radiation that have high energies and short wavelengths.

- Diffraction occurs whenever a wave encounters a series of regularly spaced obstacles that;
  - Can scatter the wave
  - Have a spacing comparable to the **wavelength**

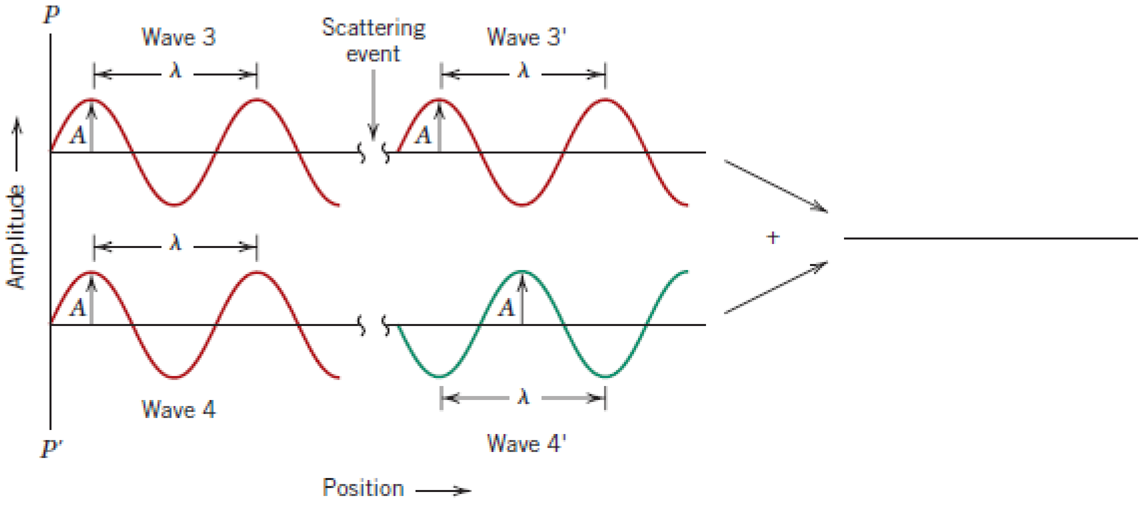
- X-ray wavelength (λ) ~ inter-atomic spacing.

- Other techniques such as neutron or electron diffraction, also, can be used.

Constructive & Destructive Interference



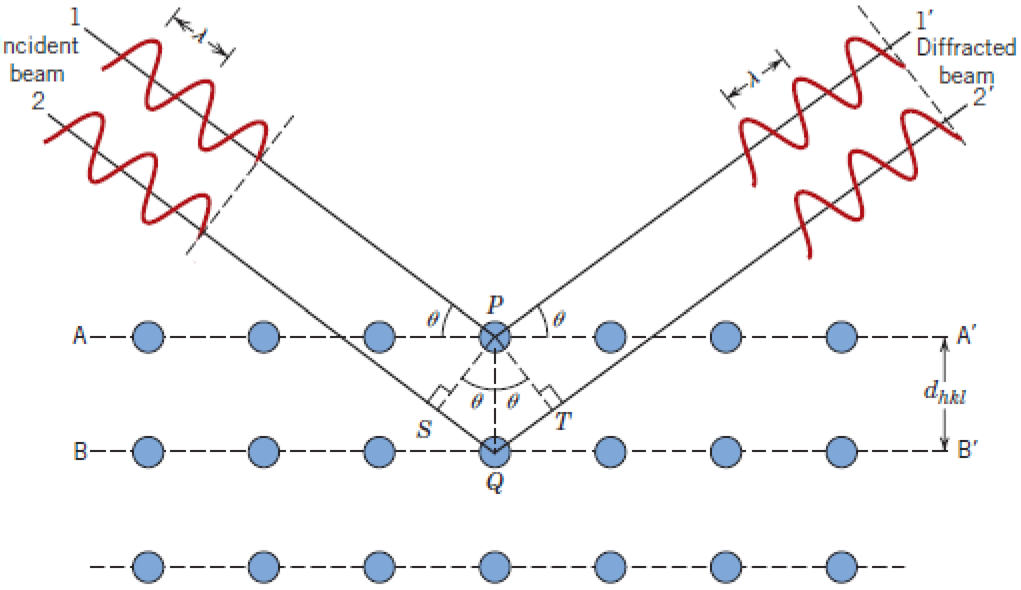
Mutually reinforce
(Constructive interface)



Destructive interface

Bragg's law

Figure 3.19
Diffraction of x-rays by planes of atoms (A–A′ and B–B′).



The law: For constructive interference, the additional path length SQ+QT must be an integer number of wavelengths (λ).

$$n\lambda = SQ + QT = d_{hkl}\sin\theta + d_{hkl}\sin\theta = 2d_{hkl}\sin\theta$$

n = 1,2,3…order of reflection

Bragg’s law

- we have a simple expression relating the x-ray wavelength and interatomic spacing to the angle of the diffracted beam.

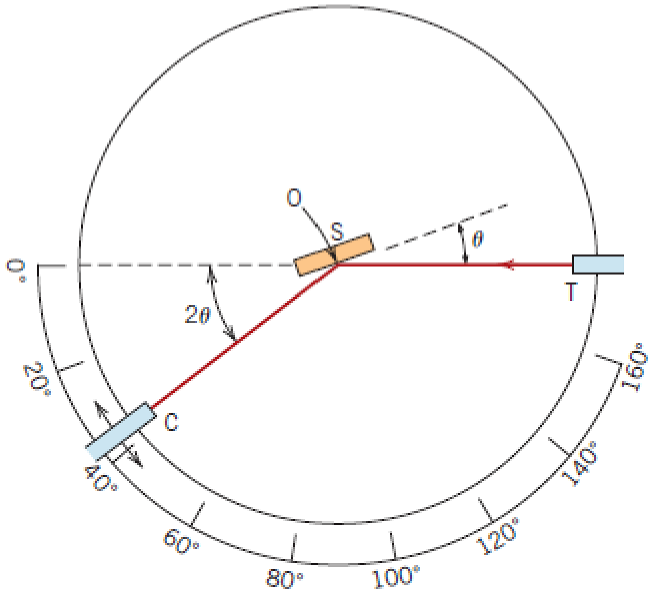
- If **Bragg’s law** is not satisfied, then the interference will be nonconstructive in nature so as to yield a very low intensity diffracted beam.

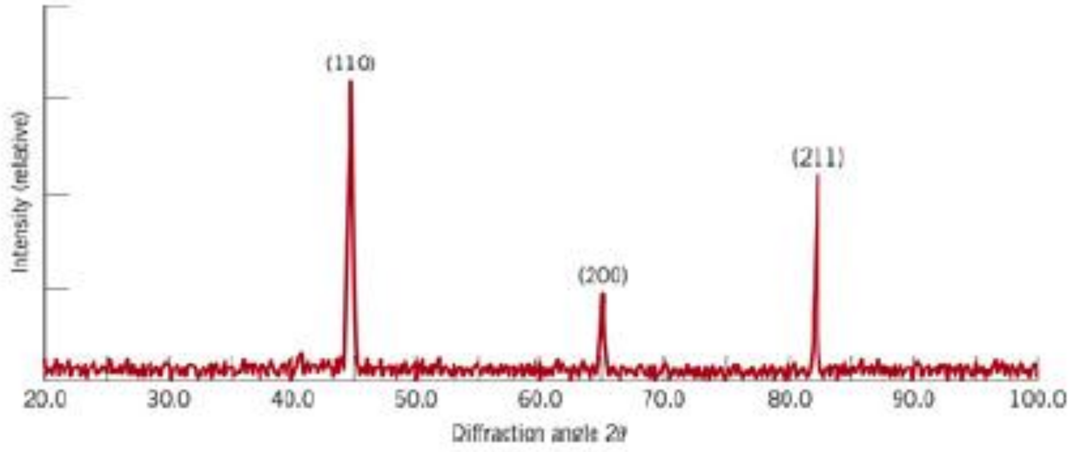
- Magnitude of difference between two adjacent and parallel planes of atoms is function of Miller Indices and the lattice parameter. For cubic symmetry:

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

Diffractometer Technique

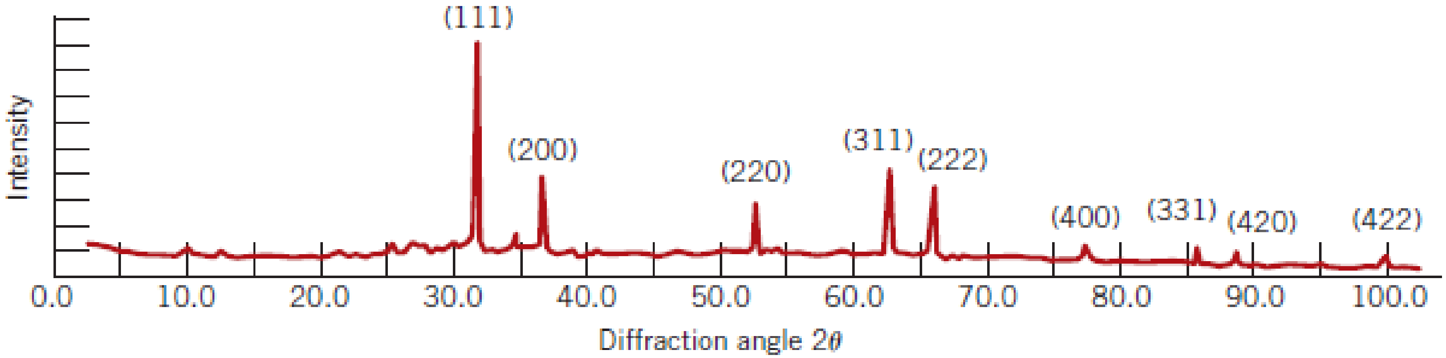
- Use powder (or polycrystalline) sample to guarantee some particles will be oriented properly such that every possible set of crystallographic planes will be available for diffraction.





Each material has a unique set of planar distances and extinctions, making X-ray diffraction useful in analysis of an unknown material

X-Ray Diffraction



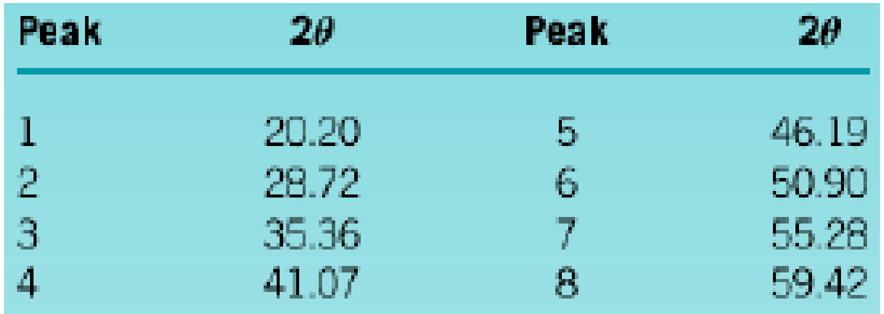
To identify the crystal structure of a material having cubic crystal system (SC, BCC or FCC). You need to look at the values of $h^2+k^2+l^2$ for the different peaks.

- If these values form a pattern of 1,2,3,4,5,6,8,.. (note 7 is missing) the structure is SC.
- **In BCC**, diffraction only occurs from planes having an even $h^2+k^2+l^2$ sum of 2,4, 6, 8, 10, 12, 14,.....etc.
- **For FCC metals**, however, more destructive interference occurs, and planes having $h^2+k^2+l^2$ sums of 3, 4, 8, 11, 12, 16, ...etc. will diffract

Examining X-ray Diffraction

The results of a x-ray diffraction experiment using x-rays with λ = 0.7107 Å (a radiation obtained from molybdenum (Mo) target) show that diffracted peaks occur at the following 2θ angles:

Determine 1) the crystal structure
2) the indices of the plane producing each peak



Peak	2θ	Peak	2θ
1	20.20	5	46.19
2	28.72	6	50.90
3	35.36	7	55.28
4	41.07	8	59.42

Use a = 2.868 Å

peak	2θ	θ	sin(θ)	d	$h^2 + k^2 + l^2$
1	20.2	10.1	0.175367	2.026325	2
2	28.72	14.36	0.248014	1.432784	4
3	35.36	17.68	0.303701	1.170067	6
4	41.07	20.535	0.35078	1.013029	8
5	46.19	23.095	0.392257	0.905911	10
6	50.9	25.45	0.429723	0.826927	12
7	55.28	27.64	0.463915	0.765981	14
8	59.42	29.71	0.49561	0.716995	16

Use a = 2.868 Å

Polymorphism and Allotropy

- Some materials may have more than one crystal structure depending on temperature and pressure - called *POLYMORPHISM*

- Carbon
  - graphite
  - diamond

- Iron BCC and FCC