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

\[ LD = \frac{n}{L_L} \]

- 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 $A_p = (AC) \times (AD)$

$AC = \ldots \ldots 4R$

$AD = \ldots a \ldots \text{where } a = 2\sqrt{2}R$

Area = $8\sqrt{2}R^2$

Number of atoms = 2 atoms

$$PD = \frac{n}{A_p} = \ldots \frac{2}{8\sqrt{2}R^2}$$
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:
  - Turbine blades
  - Nickel alloy – single crystal
  - to improve high temp. mechanical properties

- 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:

• **Polycrystals**
  - Properties may/may not vary with direction.
  - If grains are randomly oriented: **isotropic**.
  - If grains are **textured**, anisotropic.

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 ($\lambda$) ~ 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**

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

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

$n = 1, 2, 3 \ldots \text{order of reflection}$
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:

\[
d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}
\]
Diffracometer 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.
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 $\lambda = 0.7107$ Å (a radiation obtained from molybdenum (Mo) target) show that diffracted peaks occur at the following $2\theta$ angles:

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

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<th>$2\theta$</th>
<th>Peak</th>
<th>$2\theta$</th>
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Use $a = 2.868$ Å
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<th>peak</th>
<th>2θ</th>
<th>θ</th>
<th>sin(θ)</th>
<th>d</th>
<th>$h^2 + k^2 + l^2$</th>
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</table>

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