MSE200

Lecture 4 (CHAPTER 3.6-3.11)

Crystal Structures and Crystal Geometry

Instructor: Yuntian Zhu

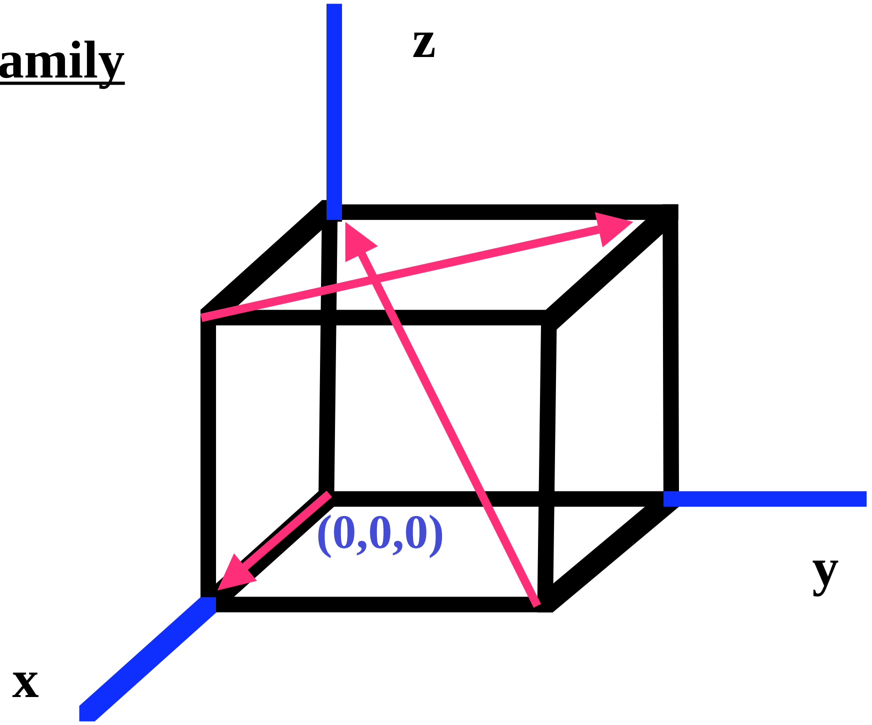
Objectives/outcomes: You will learn the following:

- List the directions of in a direction family and planes of a family
- Determine Miller's indices of planes in the cubic system
- Determine what direction lies on a plane
- Describe the atomic packing of fcc and hcp structures.
- Calculate the density from unit cells
- Calculate the planar and linear atomic densities.
- Describe X-Ray diffraction

Direction Indices in a direction family (form)

Equivalent directions: indices of a family

<uvw>:



<100> =

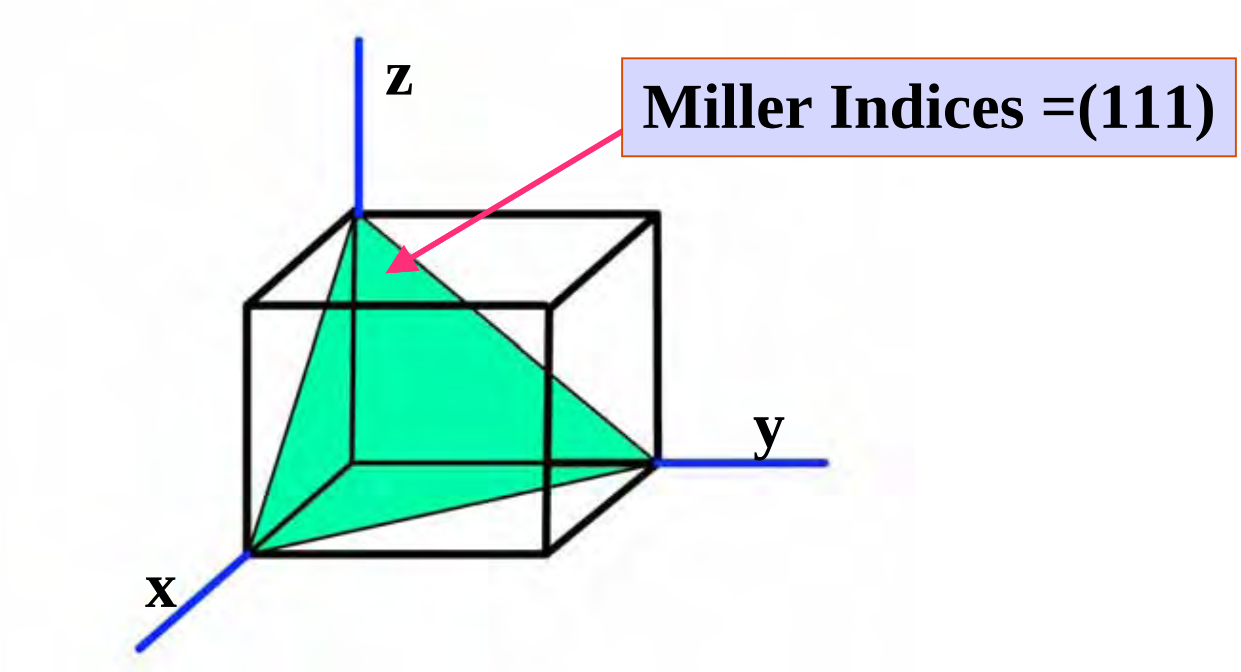
<110> =

<111> =

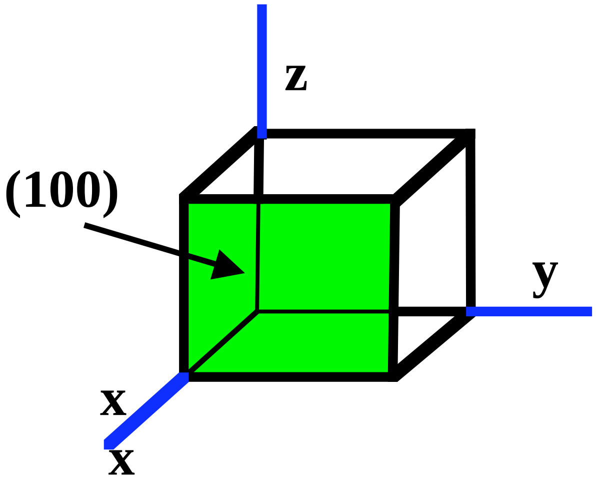
<121>=

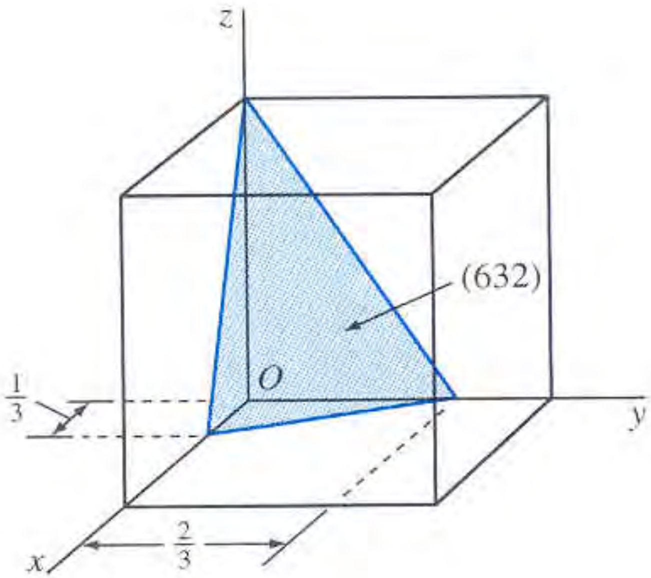
Miller Indices

- **Miller Indices: describe specific lattice planes of atoms.**



Determine Miller Indices

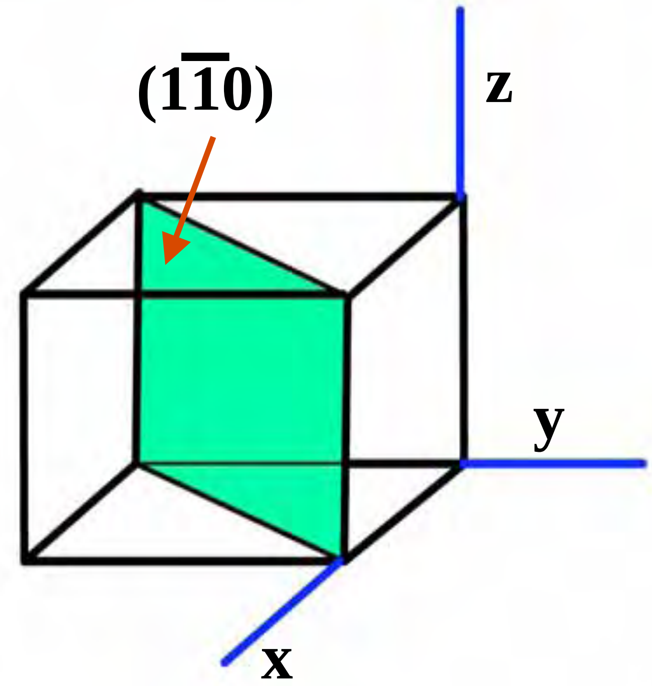




Miller Indices - Planes of a family (form)

{100} = (100), (010), (001)

{110} =

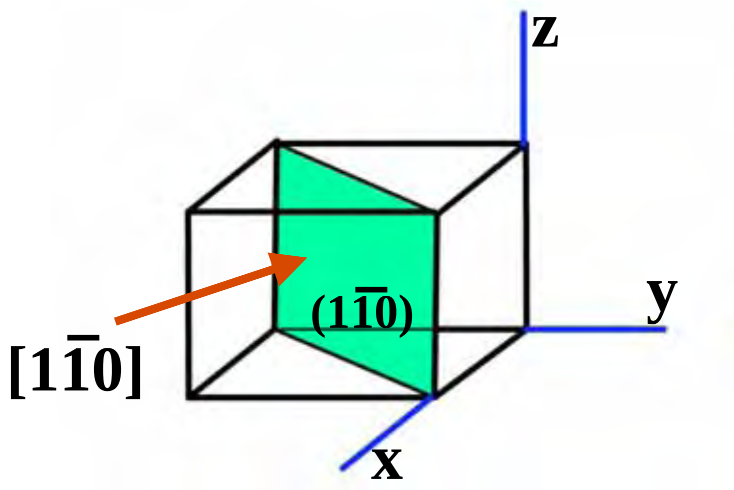


{111} =

{121}=

Miller Indices {hkl} – Important Relationship

- **Direction indices of a direction perpendicular to a crystal plane are same as miller indices of the plane.**
- Example:-

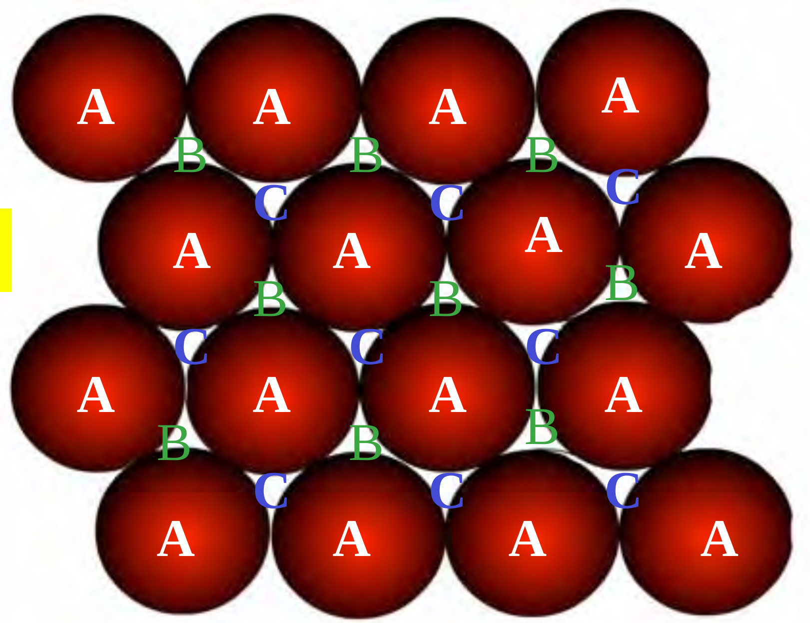


- Determine if a directions is on a plane
- **Interplanar spacing:**

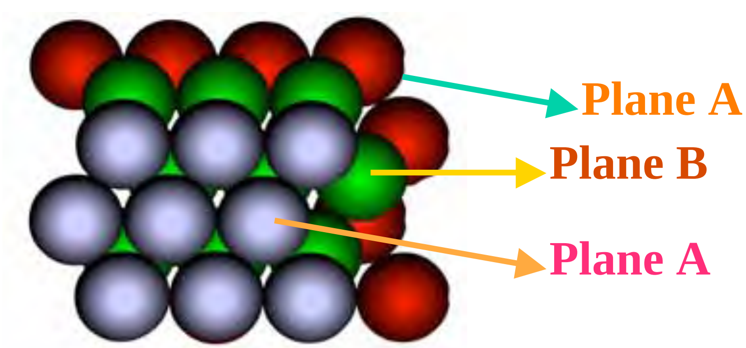
$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Structural Difference between HCP and FCC

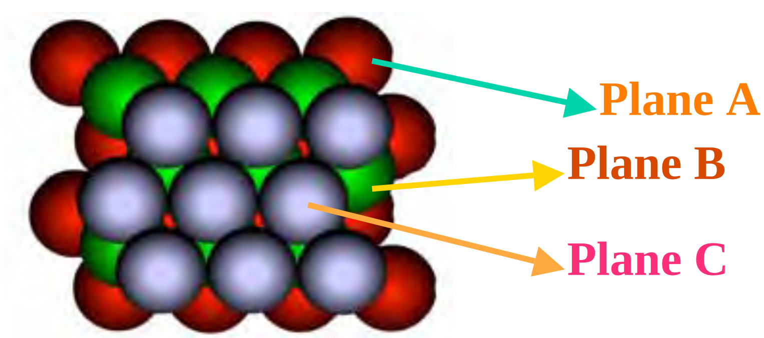
Close-packed plane



HCP packing:



FCC packing:



Volume Density

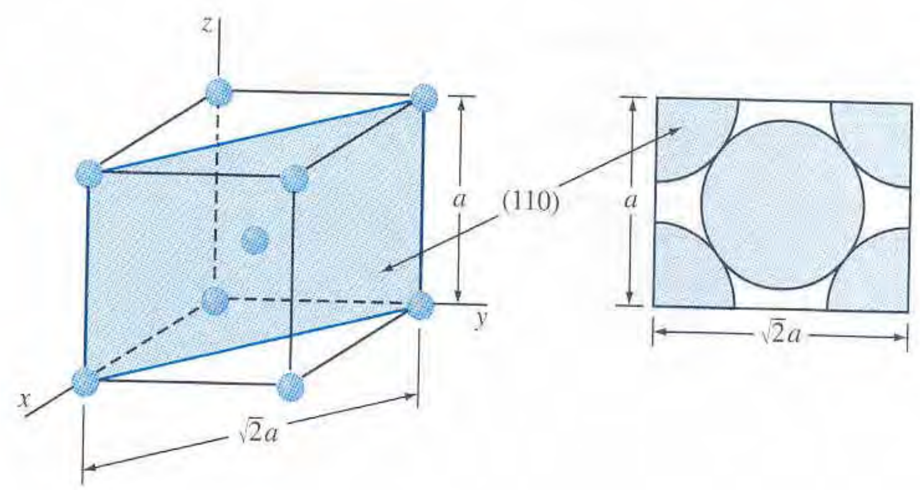
- **Volume density of metal =** ρ_v **=** $\dfrac{\textbf{Mass/Unit cell}}{\textbf{Volume/Unit cell}}$

- **Example:- Copper (FCC) has atomic mass of 63.54 g/mol and atomic radius of 0.1278 nm.**

Planar Atomic Density

- **Planar atomic density**= ρ_p = **#of atoms per unit plane area**
- **Example:- In Iron (BCC, a=0.287), The (110) plane intersects center of 5 atoms (Four ¼ and 1 full atom).**

➢



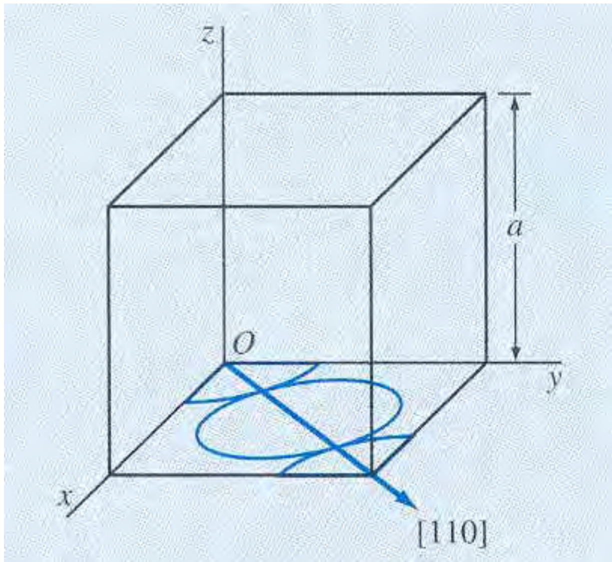
$$\rho_p = \frac{17.2 atoms}{nm^2} = \frac{1.72 \times 10^{13}}{mm^2}$$

Linear Atomic Density

- **Linear atomic density** $=\rho_l$ = **#of atoms per unit line length**

- **Example:- For a FCC copper crystal (a=0.361), the [110] direction intersects 2 half diameters and 1 full diameter.**

➢ **Therefore, it intersects ½ + ½ + 1 = 2 atomic diameters.**

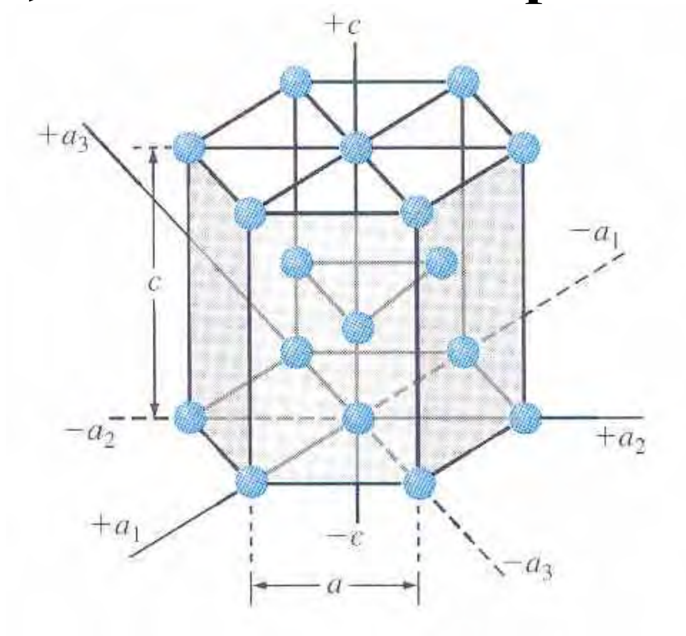


Length of line = $\sqrt{2} \times 0.361nm$

$$\rho_l = \frac{2atoms}{\sqrt{2} \times 0.361nm} = \frac{3.92atoms}{nm} = \frac{3.92 \times 10^6 atoms}{mm}$$

Planes and Directions in Hexagonal Unit Cells

- **Four indices are used (hkil) called as *Miller-Bravais* indices.**
- **Four axes are used (a_1, a_2, a_3 and c).**
- **Reciprocal of the intercepts that a crystal plane makes with the a_1, a_2, a_3 and c axes give the h,k,I and l indices respectively.**



Hexagonal Unit Cell - Examples

- **Basal Planes:-**

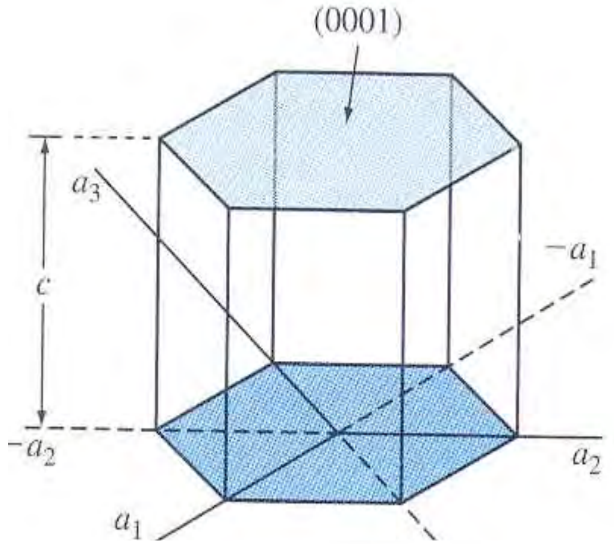
Intercepts a1 = ∞

a2 = ∞

a3 = ∞

c = 1

(hkli) = (0001)



- **Prism Planes :-**

For plane ABCD,

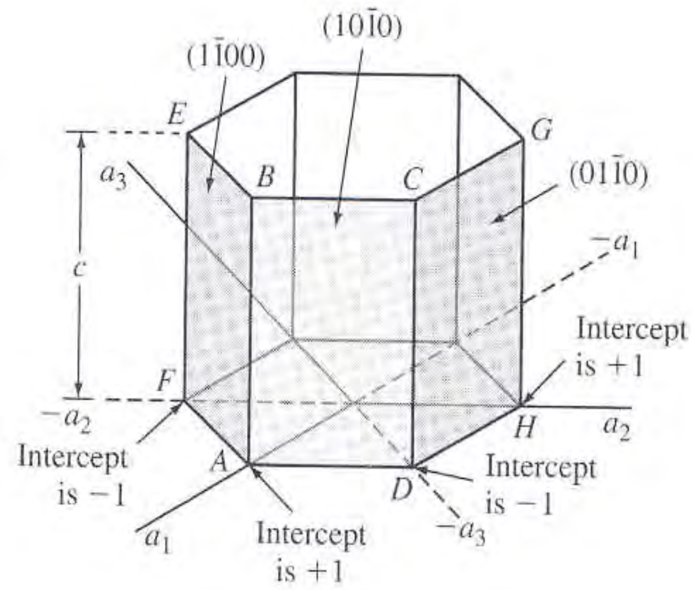
Intercepts a1 = 1

a2 = ∞

a3 = -1

c = ∞

(hkli) = (1010)

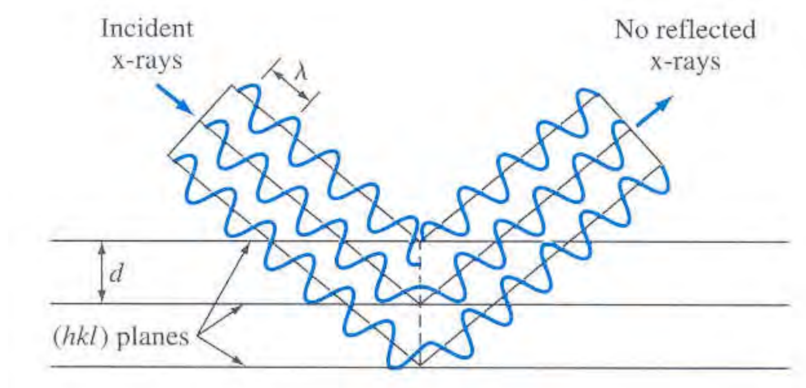


The closest packed plane and direction

- BCC: <111> {no}
- FCC: <110> {111}

X-Ray Diffraction

- **Crystal planes of target metal act as mirrors reflecting X-ray beam.**
- **Destructive interference: out of phase, no reinforced beam is produced.**



- **Constructive interference: in phase, reinforced beams are produced.**

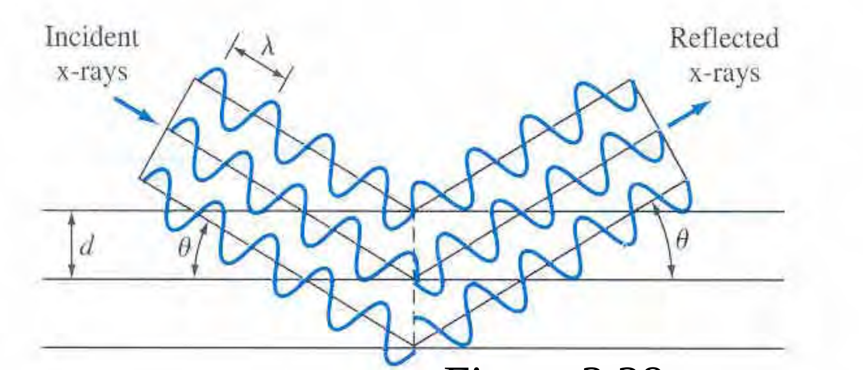


Figure 3.28

After A.G. Guy and J.J. Hren, "Elements of Physical Metallurgy," 3rd ed., Addison-Wesley, 1974, p.201)

X-Ray Diffraction (Cont..)

- For rays reflected from different planes to be in phase, the extra distance traveled by a ray should be a integral multiple of wave length λ .

$$n\lambda = 2\, d_{hkl}.\text{Sin}\theta$$

(n = 1,2…)

n is order of diffraction

d_{hkl} is interplanar distance,

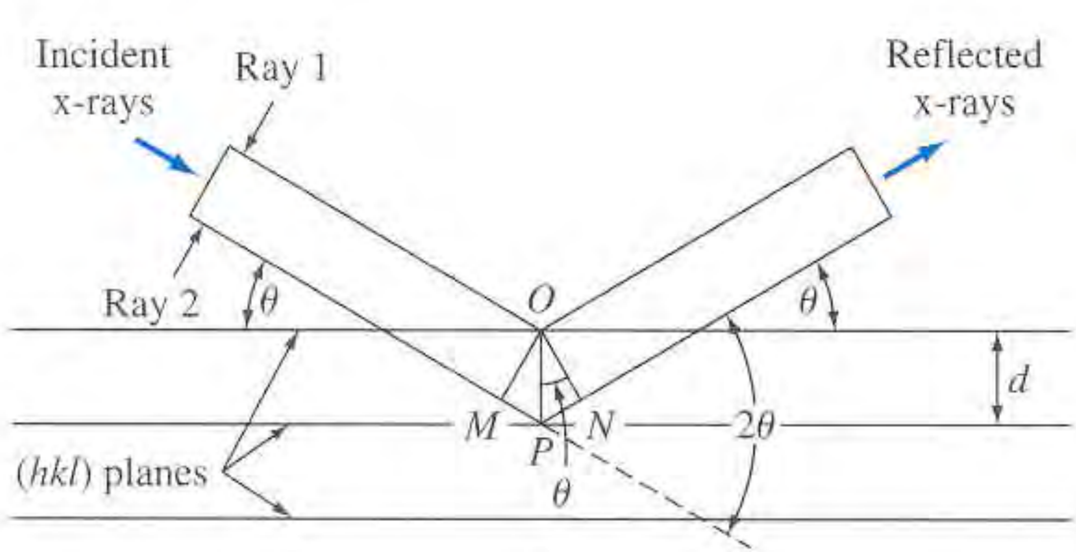
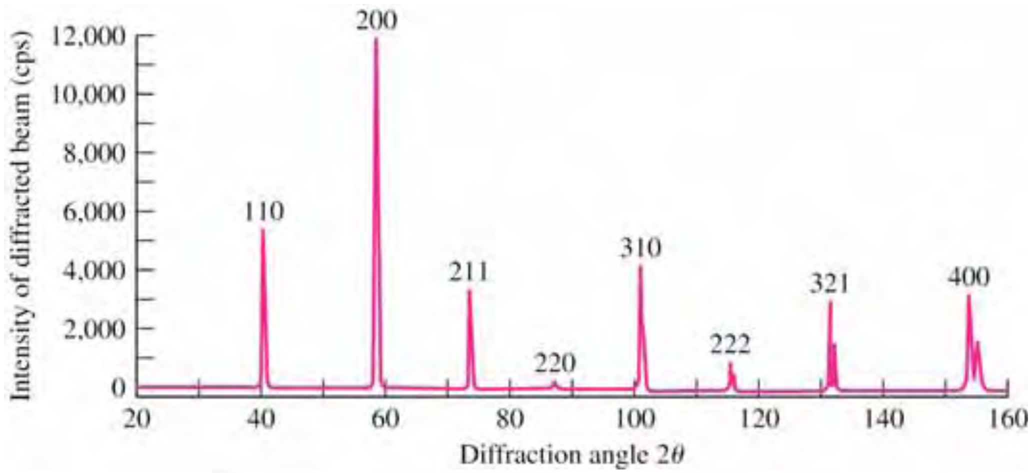


Figure 3.28

$$\lambda = 2\, d_{hkl}.\text{Sin}\theta$$

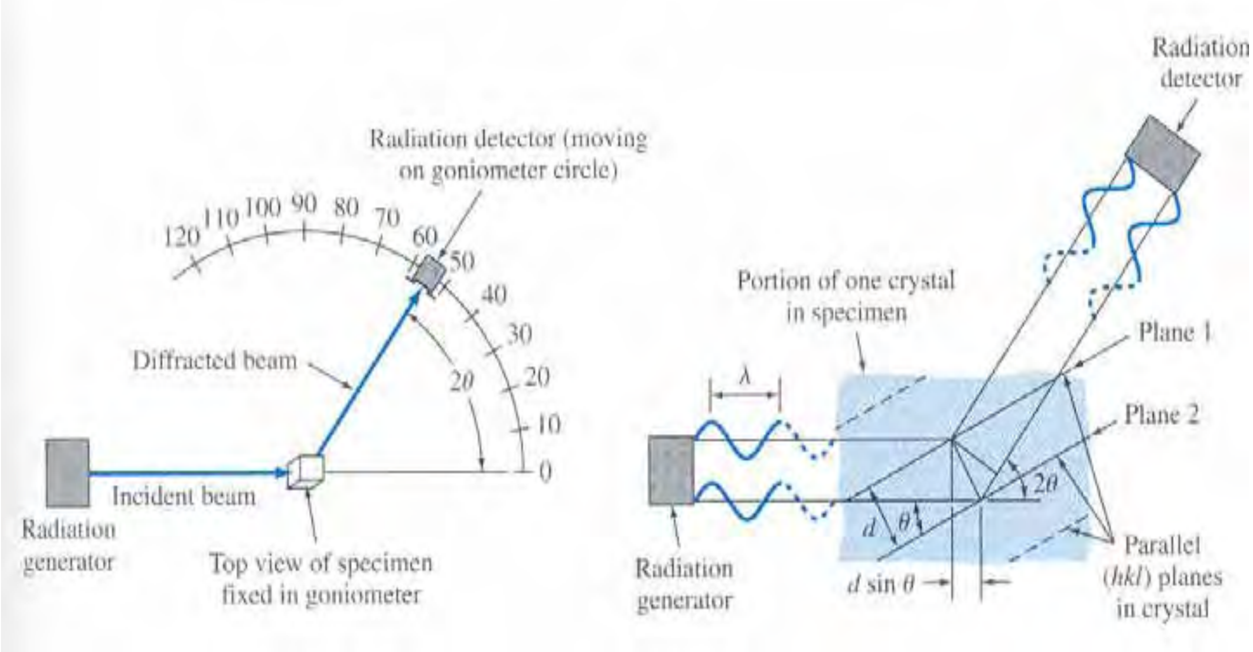
After A.G. Guy and J.J. Hren, "Elements of Physical Metallurgy," 3d ed., Addison-Wesley, 1974, p.201.)

Interpreting Diffraction Data



$$\lambda = 2dSin\theta$$

$$Sin^2\theta = \frac{\lambda^2(h^2+k^2+l^2)}{4a^2}$$



 http://www.mse.ncsu.edu/research/zhu/ Department of Materials Sci. & Eng.

Homework

Example Problems: 3.7, 3.8, 3.9, 3.10, 3.11,
Regular Problems, Chapter 3: 38, 39, 40, 41, 43, 4446, 47, 48, 49, 50,51, 52, 54,56, 57, 58, 59, 69,70,71, 72,
Reading assignment for the next class: 4.3-4.4