Miller Indices **Lec 4**

- Miller indices are used to specify directions and planes.
- These directions and planes could be in lattices or in crystals.
- The number of indices will match with the dimension of the lattice or the crystal.
- (h,k,l) represents a point – note the exclusive use of commas
- Negative numbers/directions are denoted with a bar on top of the number
- [hkl] represents a direction [x,y,z]
- (hkl) represents a plane (1/x, 1/y, 1/z)*1/CM
- {hkl} represents a family of planes.

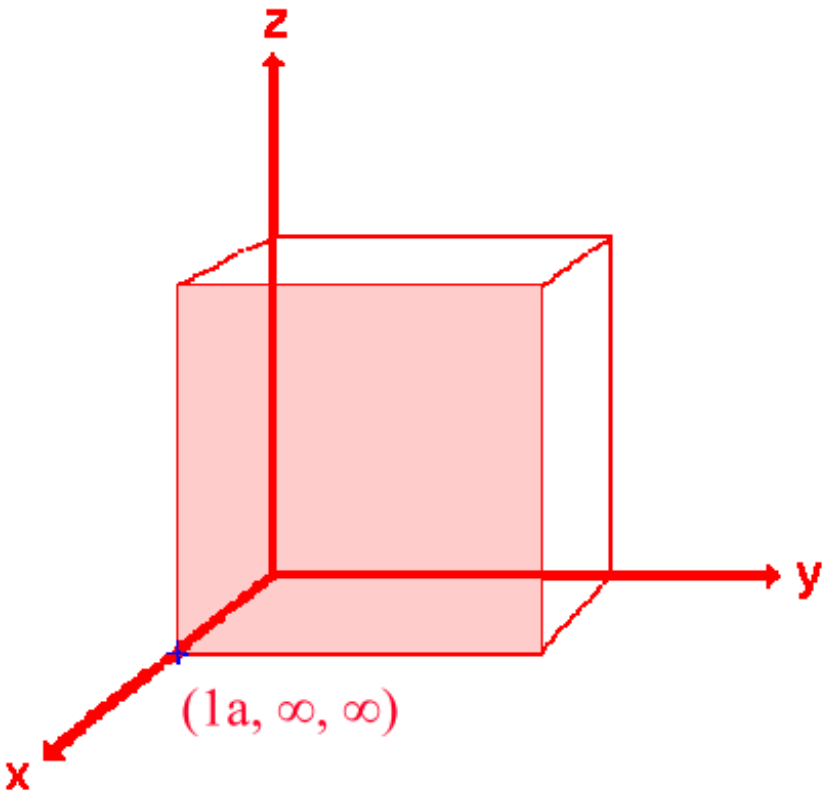
Miller Indices for Directions

Miller Indices for Directions

1. Identify the plane intercepts on the x, y and z-axes. 2. Specify intercepts in fractional coordinates. 3. Take the reciprocals of the fractional

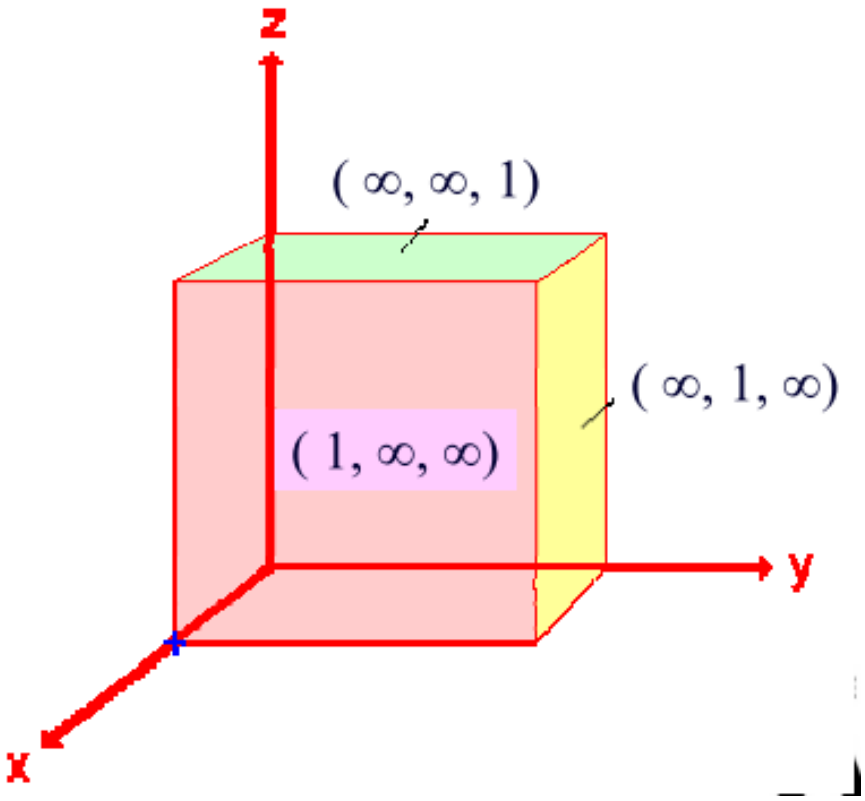
intercepts.

The plane intersects the x-axis at point a. It runs parallel along y and z axes. Thus, this plane can be designated as (1,∞,∞)



Miller Indices

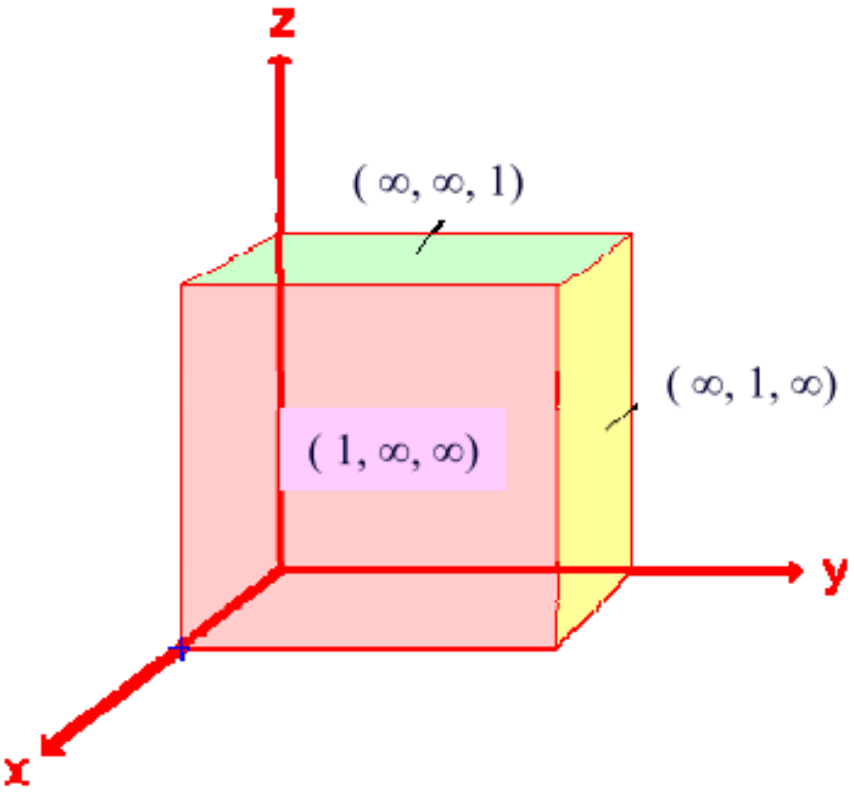
• Likewise, the yellow plane can be designated as (∞,1,∞) • And the green plane can be written as (∞,∞,1)



3

Miller Indices

- Miller Indices are the reciprocals of the parameters of each crystal face. Thus:
- Pink Face = (1/1, 1/∞, 1/∞) = (100)
- Green Face = (1/∞, 1/∞, 1/1) = (001)
- Yellow Face = (1/∞, 1/1, 1/∞) = (010)



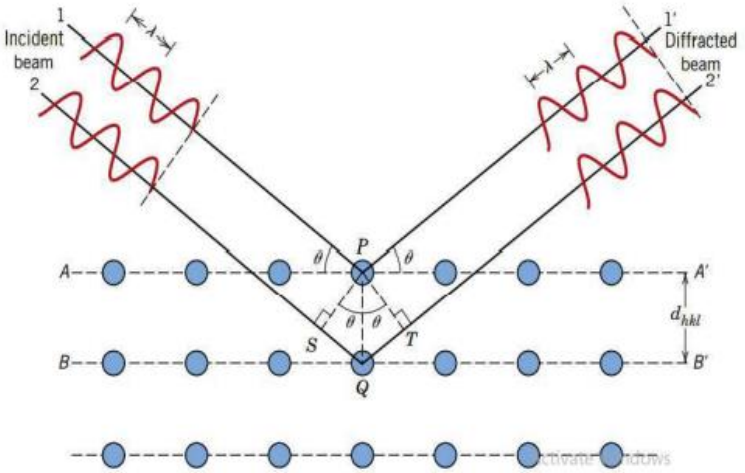
Importance of Miller Indices

- In Materials Science it is important to have a notation system for atomic planes since these planes influence
- Optical properties
- Reactivity
- Surface tension
- Dislocations

5

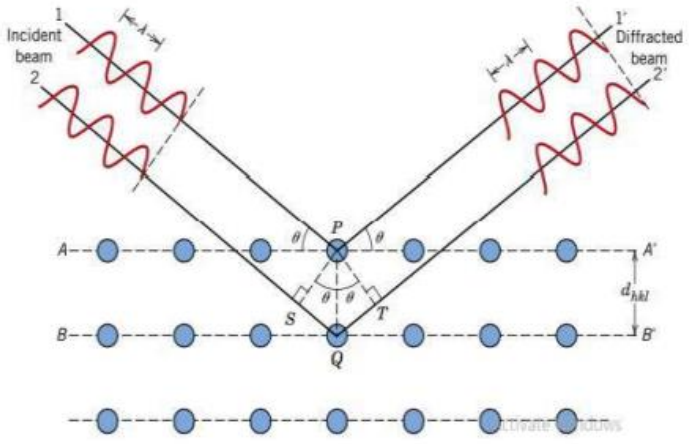
X-rays Diffraction

- Consider the two parallel planes of atoms $A - A'$ and $B - B'$ in Figure below which have the same $h, k, \text{and } l$ Miller indices and are separated by the interplanar spacing d_{hkl}



- if the path length difference between $1-P-1'$ and $2-Q-2'$ (i.e., $\overline{SQ} + \overline{QT}$) is equal to a whole number, n, of wavelengths that is, the condition for diffraction is:

$$n\lambda = \overline{SQ} + \overline{QT} \qquad \ldots\ldots\ldots (3.20)$$

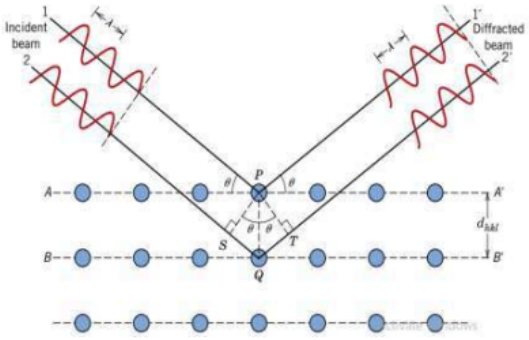


$$n\lambda = d_{hkl} \sin\theta + d_{hkl} \sin\theta$$

$$n\lambda = 2d_{hkl} \sin\theta \ldots\ldots\ldots (3.21)$$

Equation 3.21 is known as **Bragg's law**

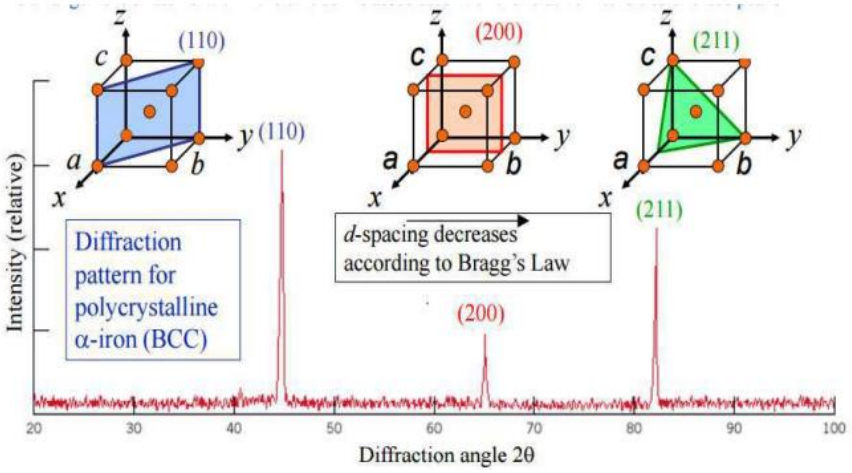
n is the order of reflection, which may be any integer (1, 2, 3, . . .) consistent with $\sin\theta$ not exceeding unity.



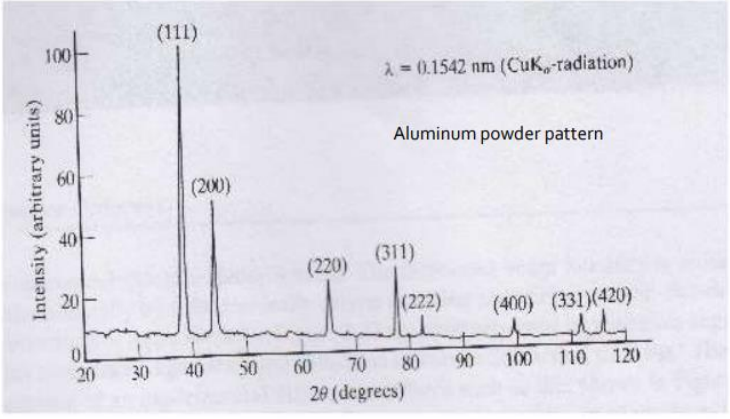
- Bragg's law expression relating the x-ray wavelength and interatomic spacing to the angle of the diffracted beam.

$$n\lambda = 2d_{hkl} \sin\theta \ldots\ldots\ldots (3.21)$$

- For the BCC crystal structure, $h + k + l$ must be even if diffraction is to occur



- for FCC, $h, k,$ and l must all be either odd or even



- ***reflection rules***, are summarized in Table below
- Zero is considered to be an even integer

Crystal Structure	*Reflections Present*	*Reflection Indices for First Six Planes*
BCC	$(h + k + l)$ even	110, 200, 211, 220, 310, 222
FCC	h, k, and l either all odd or all even	111, 200, 220, 311, 222, 400
Simple cubic	All	100, 110, 111, 200, 210, 211

Inter-planar atomic distance

- The magnitude of the distance between two adjacent and parallel planes of atoms (i.e., the interplanar spacing d_{hkl}) is a function of the Miller indices ($h, k,$ and l) as well as the lattice parameter(s).

For example, for crystal structures that have cubic symmetry,

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad \ldots\ldots\ldots (3.22)$$

a is the lattice parameter (unit cell edge length).

- Relationships similar to Equation 3.22, but more complex, exist for the other six crystal systems

Orthorhombic	Tetragonal	Cubic
$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$	$\frac{1}{d_{hkl}^2} = \left[h^2 + k^2 + l^2\left(\frac{a}{c}\right)^2\right]\frac{1}{a^2}$	$\frac{1}{d_{hkl}^2} = (h^2 + k^2 + l^2)\frac{1}{a^2}$
Monoclinic		**Hexagonal**
$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2 \sin^2\gamma} + \frac{k^2}{b^2 \sin^2\gamma} - \frac{2hk\cos\gamma}{ab\sin^2\gamma} + \frac{l^2}{c^2}$		$\frac{1}{d_{hkl}^2} = \left[\frac{4}{3}(h^2 + k^2 + hk) + l^2\left(\frac{a}{c}\right)^2\right]\frac{1}{a^2}$

Inter-planar atomic distance

EXAMPLE PROBLEM
Interplanar Spacing and Diffraction Angle Computations

For BCC iron, compute **(a)** the interplanar spacing and **(b)** the diffraction angle for the (220) set of planes. The lattice parameter for Fe is 0.2866 nm. Assume that monochromatic radiation having a wavelength of 0.1790 nm is used, and the order of reflection is 1.

Solution

(a)

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad \ldots\ldots\ldots (3.22)$$

$$d_{hkl} = \frac{0.2866\ nm}{\sqrt{2^2 + 2^2 + 0^2}} = 0.1013\ m$$

(b)

$$n\lambda = 2d_{hkl} \sin\theta \ \ldots\ldots\ldots (3.21)$$

$$\sin\theta = \frac{n\lambda}{2d_{hkl}} = \frac{1 \times 0.1790\ \text{nm}}{2 \times 0.1013\ \text{nm}} = 0.884$$

$$\theta = \sin^{-1}(0.884\ ) = 62.13^{\circ}$$

The diffraction angle is 2θ, or

$$2\theta = 2 \times 62.13^{\circ} = 124.26^{\circ}$$

EXAMPLE PROBLEM
Interplanar Spacing and Diffraction Angle Computations

X rays from a copper X-ray tube (λ = 154 pm) were diffracted at an angle of 14.20 degrees by a crystal. Assuming first-order diffraction (n = 1 in the Bragg equation), what is the interplanar spacing in this crystal?

Solution

Bragg's law says:

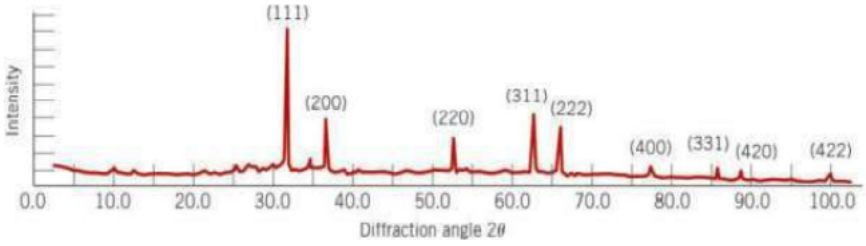
2dsinθ = nλ, where d is interplanar spacing

$$d = \frac{n\lambda}{2\sin\theta} = \frac{154}{2 \times 0{,}245} = 314\ \text{pm}$$

Inter-planar atomic distance

EXAMPLE PROBLEM
Interplanar Spacing and Lattice Parameter Computations for Lead

Figure 3.24 shows an x-ray diffraction pattern for lead taken using a diffractometer and monochromatic x-radiation having a wavelength of 0.1542 nm; each diffraction peak on the pattern has been indexed. Compute the interplanar spacing for each set of planes indexed; also, determine the lattice parameter of Pb for each of the peaks. For all peaks, assume the order of diffraction is 1



Solution

For each peak, in order to compute the interplanar spacing and the lattice parameter we must employ Equations 3.21 and 3.22, respectively. The first peak of Figure 3.24, which results from diffraction by the (111) set of planes, occurs at $2\theta = 31.3°$; the corresponding interplanar spacing for this set of planes, using Equation 3.21, is equal to

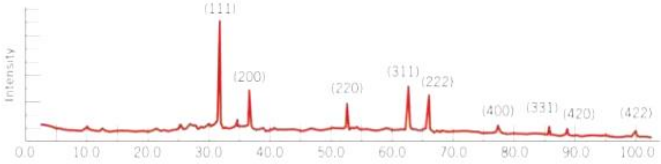
$$d_{111} = \frac{n\lambda}{2\sin\theta} = \frac{(1)(0.1542\text{ nm})}{(2)\left[\sin\left(\frac{31.3°}{2}\right)\right]} = 0.2858\text{ nm}$$

And, from Equation 3.22, the lattice parameter a is determined as

$$\begin{aligned} a &= d_{hkl}\sqrt{h^2 + k^2 + l^2} \\ &= d_{111}\sqrt{(1)^2 + (1)^2 + (1)^2} \\ &= (0.2858\text{ nm})\sqrt{3} = 0.4950\text{ nm} \end{aligned}$$

Similar computations are made for the next four peaks; the results are tabulated below:

Peak Index	*2θ*	*d_{hkl}(nm)*	*a(nm)*
200	36.6	0.2455	0.4910
220	52.6	0.1740	0.4921
311	62.5	0.1486	0.4929
222	65.5	0.1425	0.4936



Example about solidification time

1. In the casting of steel under certain mold conditions, the mold constant in Chvorinov's Rule is known to be **4.0 min/cm^2**, based on previous experience. The casting is a **flat plate** (fig. 1) whose length **l= 30 cm,** width **w= 10 cm,** and thickness **h= 20 mm.** Determine how long it will take for the casting to solidify.

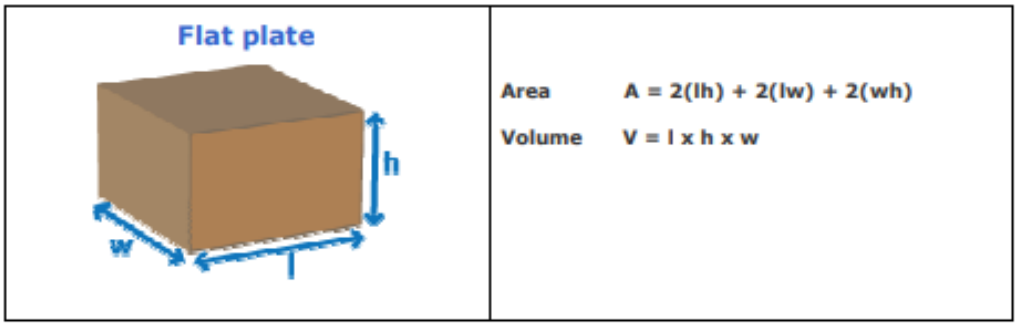


Figure 1

Solution:

Area $A = 2(30 \times 10) + 2(30 \times 2) + 2(10 \times 2) = 760\ cm^2$

Volume $V = 30 \times 10 \times 2 = 600\ cm^3$

Chvorinov's Rule: $T_{TS} = C_m(V/A)^2 = 4(600/760)^2 =$ **2.49 min**

Example about solidification time

2. A **cylindrical-shaped part** (fig. 2) is to be cast out of aluminum. The radius of the cylinder **r= 250 mm** and its thickness **h= 20 mm**. If the mold constant C_m **= 2.0 sec/mm^2** in Chvorinov's Rule, how long will it take the casting to solidify?

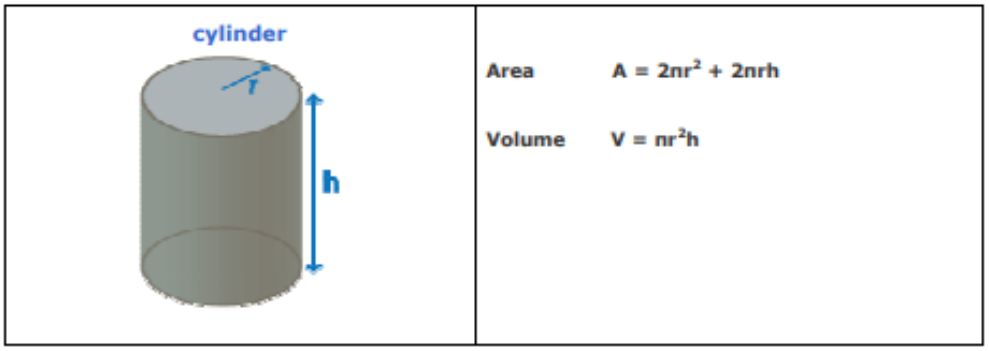


Figure 2

Solution:

Area $A = 2\,\pi\, r^2 + 2\pi\, r\, h = 2\,\pi\,(250)^2 + 2\pi\,(250)\,(20) = 424{,}115\ mm^2$

Volume $V = \pi\, r^2\, h = \pi\,(250)^2\,(20) = 3{,}926{,}991\ mm^3$

Chvorinov's Rule: $T_{TS} = C_m\,(V/A)^2 = 2\,(3{,}926{,}991 / 424{,}115)^2 =$ **171.5 s = 2.86 min**