Atomic Packing Factor

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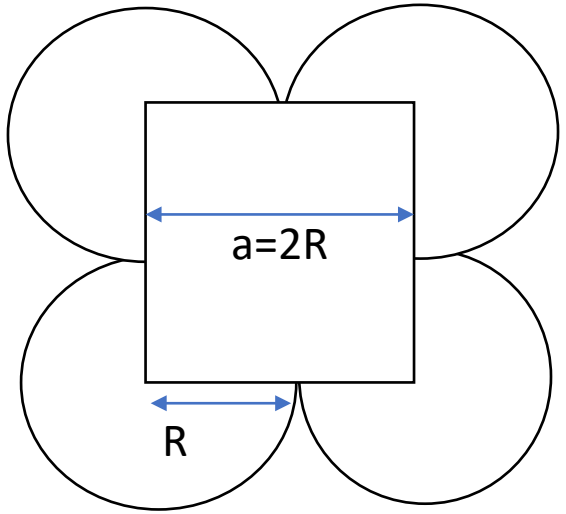
Atomic Packing Factor Calculation

- APF=Volume of atoms in unit cell/Total unit cell volume

APF Calculation Task

- Calculate A.P.F of Simple Cubic Crystal



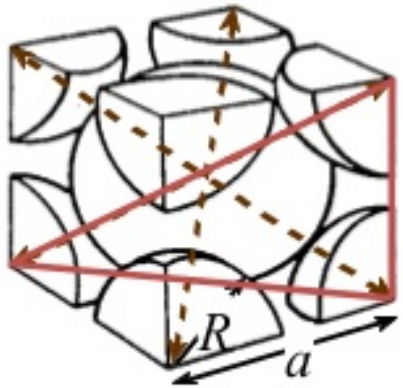
APF=Volume of Atoms/Volume of unit cell

=(1 *(4/3)*pi()*R^3)/a^3

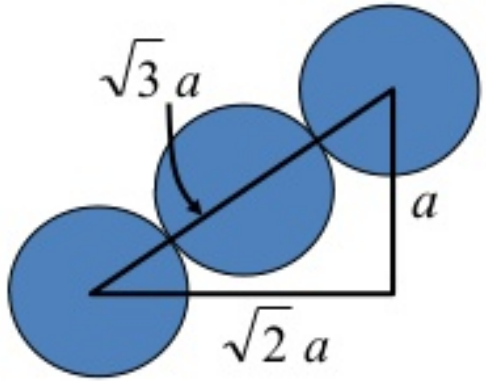
= (4/3)*pi()*R^3/8R^3

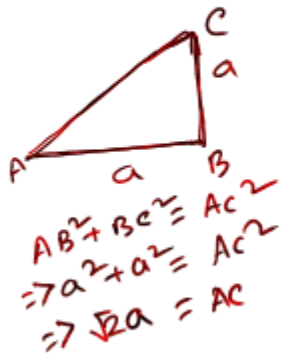
=0.52

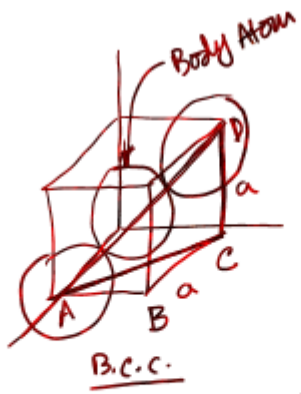
Atomic Packing Factor (APF) for BCC

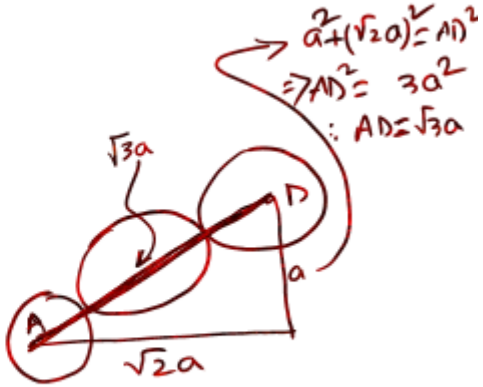


Adapted from
Fig. 3.2(a), *Callister 7e.*









Step 1: Number of atoms per unit cell =
1 atom at center + 1/8 th of 8 corner atoms = 2 atoms

Step 2: Identify close packed direction

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

Step 3: Volume of unit cell $= a^3 = \left(\frac{4R}{\sqrt{3}}\right)^3$

$$\textbf{Atomic Packing Factor} = \frac{\textbf{Volume of atoms}}{\textbf{Volume of unit cell}} = \frac{2x\frac{4}{3}\pi R^3}{a^3} = 0.68$$

Crystal Point, Direction and Plane

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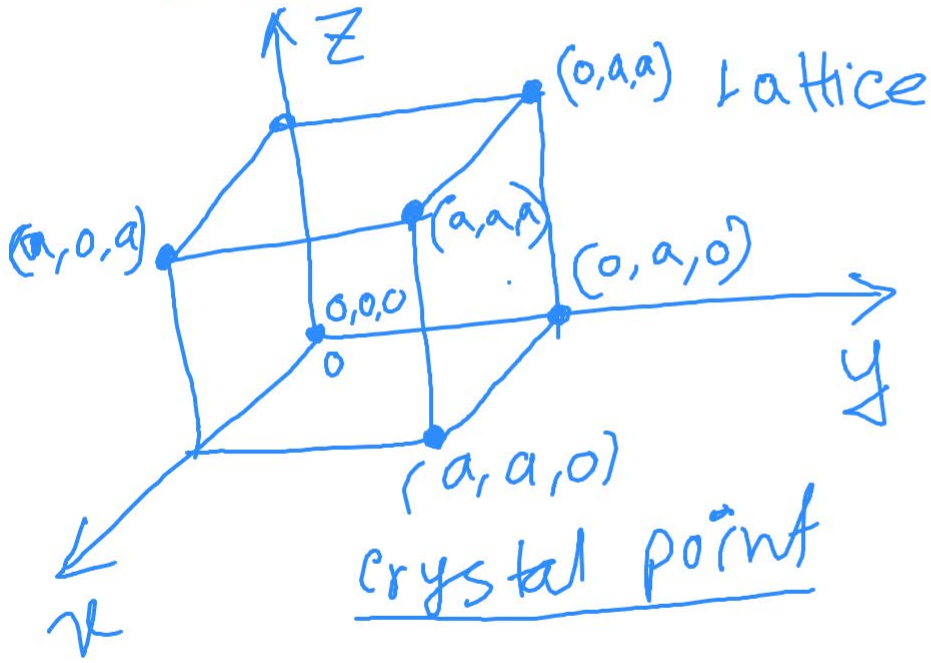
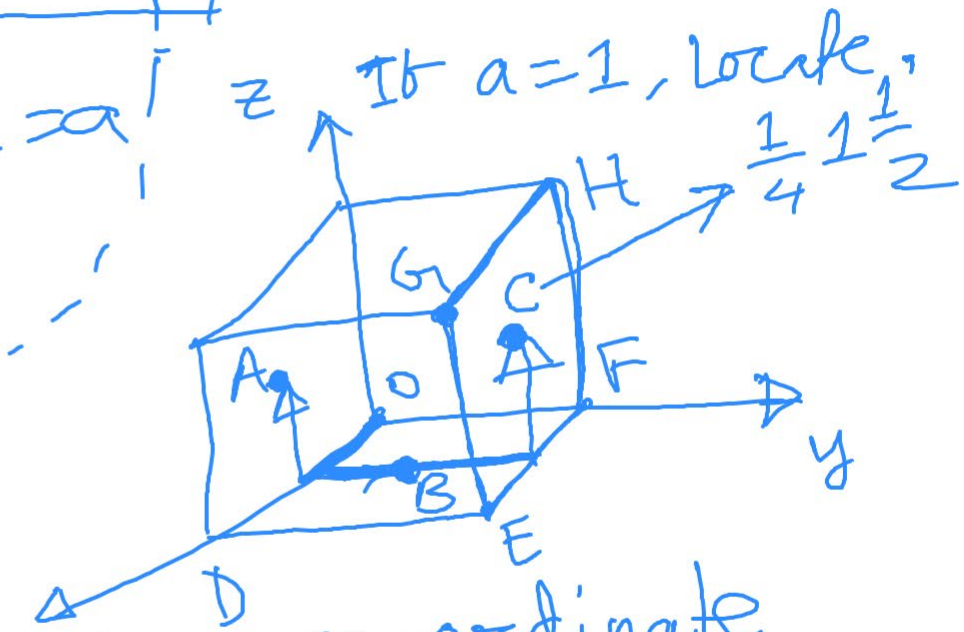
Crystal point, Directions and planes



Crystal point

Lattice parameter = a

(x, y, z)

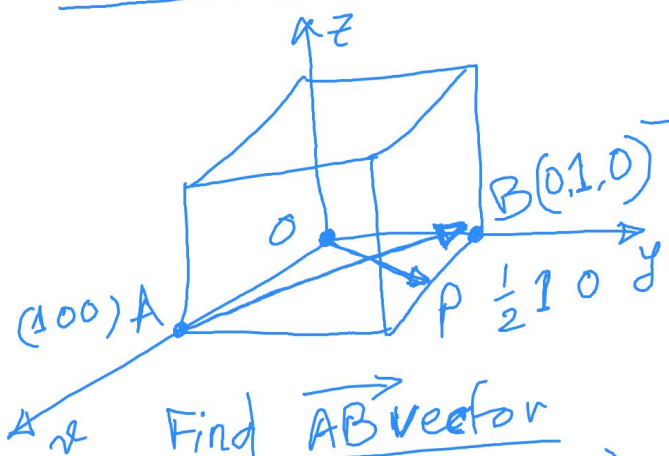


Co-ordinate

$(\underset{x}{\frac{1}{2}}, \underset{y}{1}, \underset{z}{\frac{1}{2}}) \Rightarrow A = \frac{1}{2}, 0, \frac{1}{2}$

Crystallographic Directions

crystallographic Directions → Direction Indices



Procedure:

	x	y	z	
Projection	½	1	0	
origination	0	0	0	
Reduction	½	1	0	× 2
Enclosure	[1	2	0]	

$\overrightarrow{OP} \rightarrow [120]$

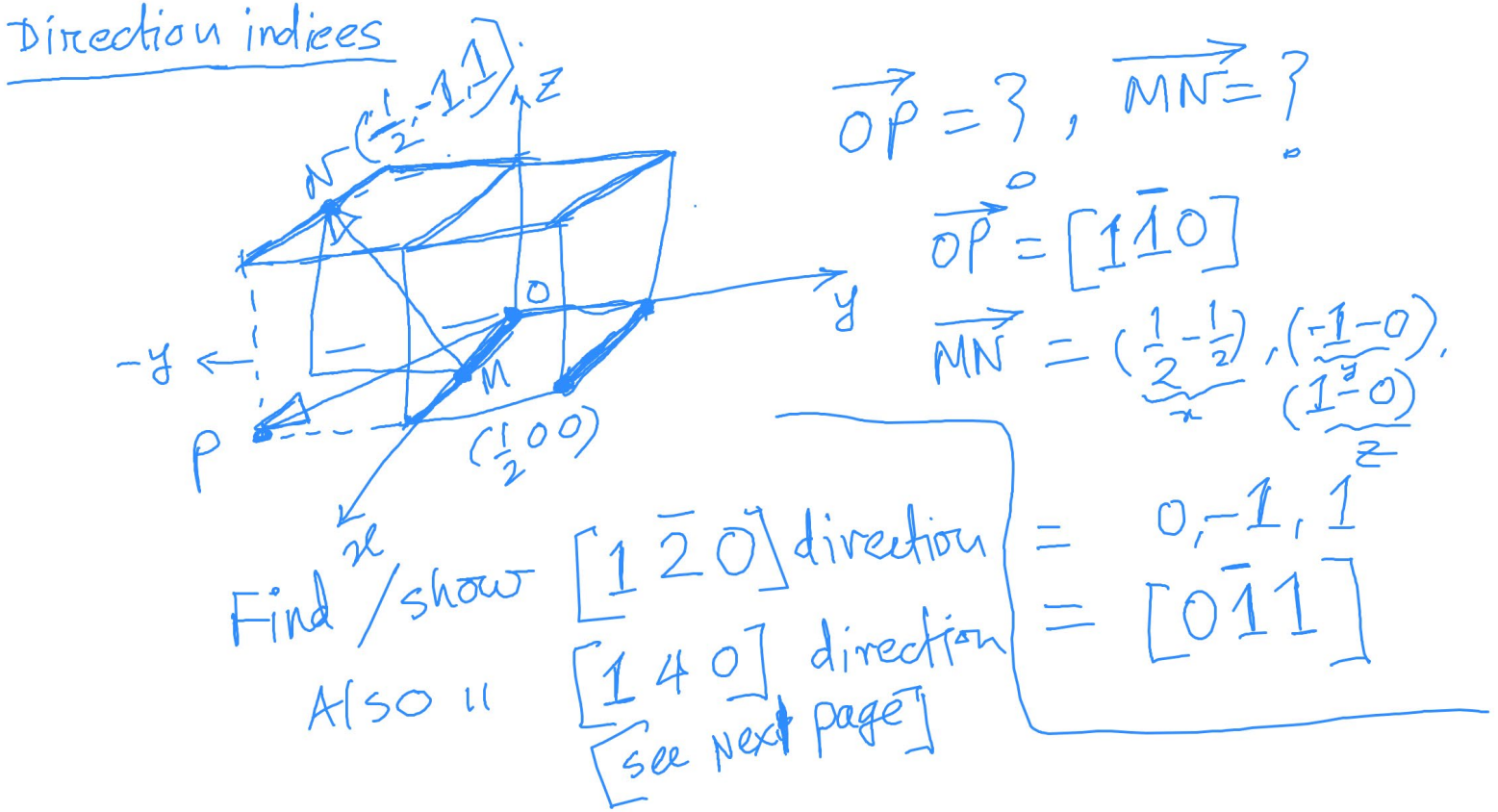
Find $\overrightarrow{AB}$ vector

$\overrightarrow{AB}$ (0−1).(1−0)(0−0)

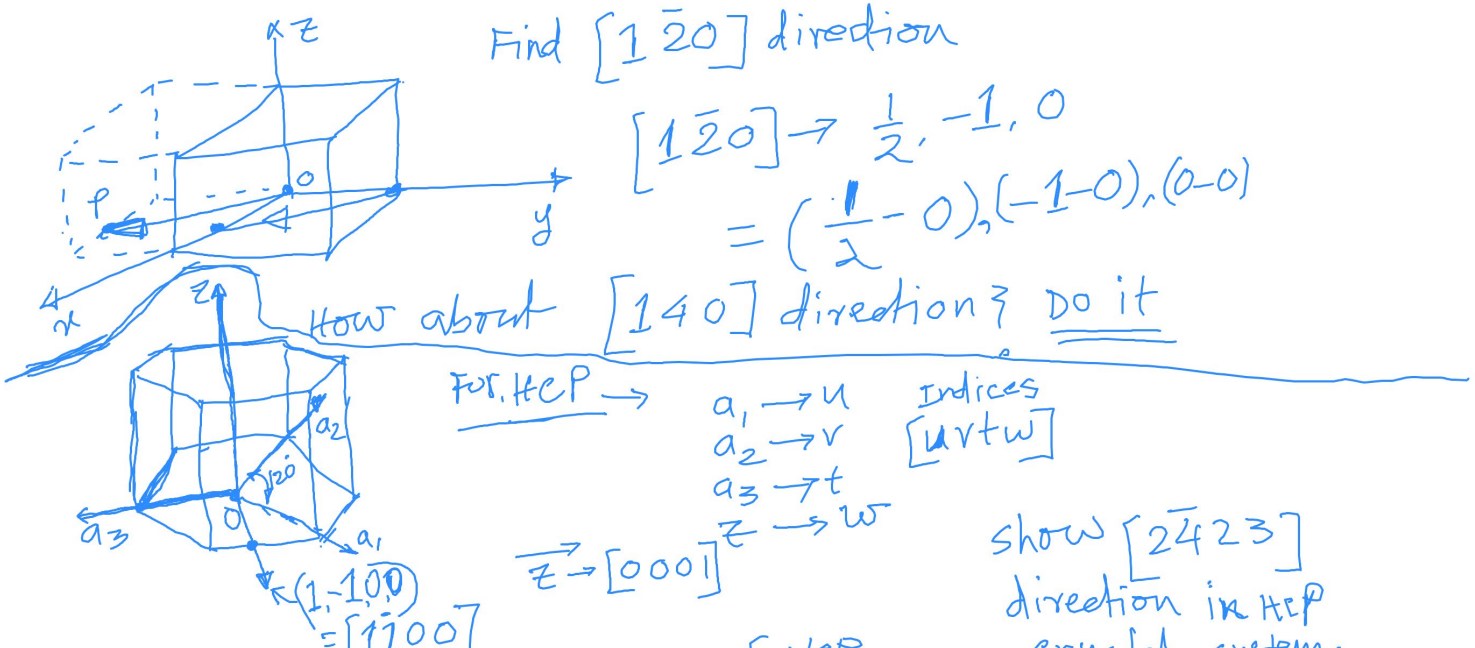
= −1 1 0

Enclose → $\overrightarrow{AB}$ $[\bar{1}10]$

Direction Indices



Direction Indices Calculation



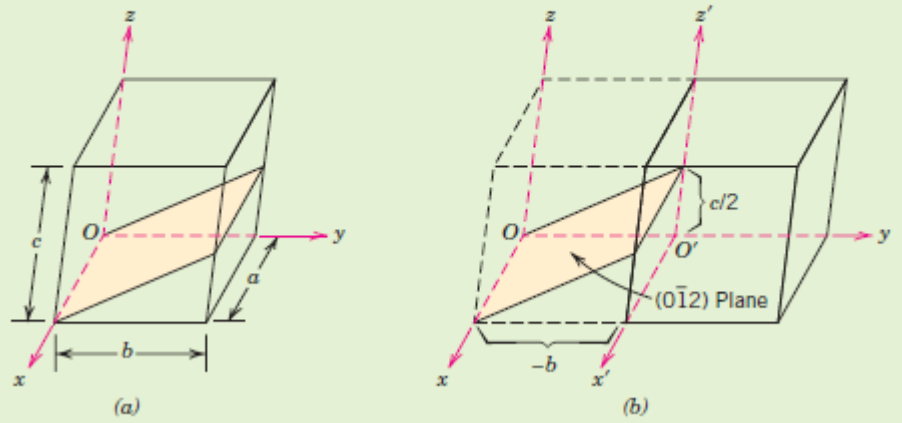
Miller Indices: Indices of Crystal Plane

- Read the Addendum on Miller Indices included in Open Lab

Example on Miller Indices

Determination of Planar (Miller) Indices

Determine the Miller indices for the plane shown in the accompanying sketch (*a*).



Solution

Because the plane passes through the selected origin O, a new origin must be chosen at the corner of an adjacent unit cell, taken as O' and shown in sketch (*b*). This plane is parallel to the x axis, and the intercept may be taken as ∞a. The y and z axes' intersections, referenced to the new origin O', are $-b$ and $c/2$, respectively. Thus, in terms of the lattice parameters a, b, and c, these intersections are ∞, -1, and $\frac{1}{2}$. The reciprocals of these numbers are 0, -1, and 2; because all are integers, no further reduction is necessary. Finally, enclosure in parentheses yields (0$\bar{1}$2).

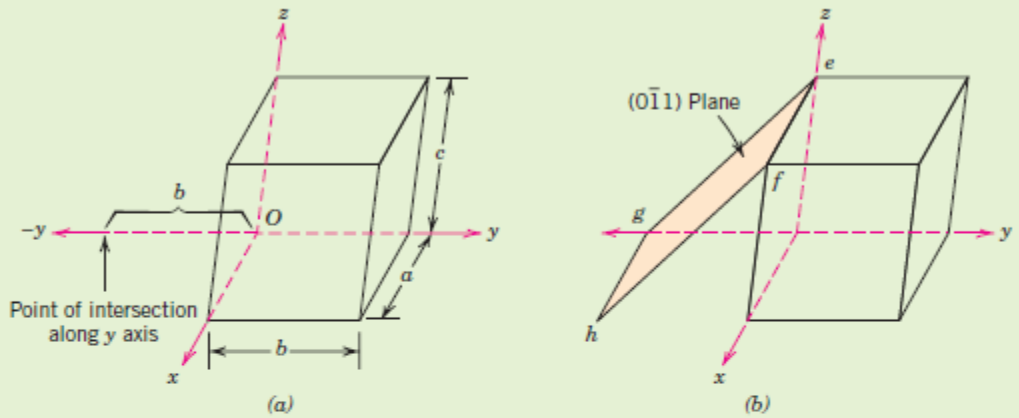
These steps are briefly summarized here:

	x	*y*	*z*
Intercepts	∞a	$-b$	$c/2$
Intercepts (in terms of lattice parameters)	∞	-1	$\frac{1}{2}$
Reciprocals	0	-1	2
Reductions (unnecessary)			
Enclosure		(0$\bar{1}$2)	

Construction of a Specified Plane

Construction of Specified Crystallographic Plane

Construct a $(0\bar{1}1)$ plane within a cubic unit cell.



Solution

To solve this problem, carry out the procedure used in the preceding example in reverse order. To begin, the indices are removed from the parentheses, and reciprocals are taken, which yields ∞, -1, and 1. This means that the particular plane parallels the x axis while intersecting the y and z axes at $-b$ and c, respectively, as indicated in the accompanying sketch (a). This plane has been drawn in sketch (b). A plane is indicated by lines representing its intersections with the planes that constitute the faces of the unit cell or their extensions. For example, in this figure, line ef is the intersection between the $(0\bar{1}1)$ plane and the top face of the unit cell; also, line gh represents the intersection between this same $(0\bar{1}1)$ plane and the plane of the bottom unit cell face extended. Similarly, lines eg and fh are the intersections between $(0\bar{1}1)$ and back and front cell faces, respectively.

X-Ray Diffraction and Bragg's Law

Consider the two parallel planes of atoms A–A' and B–B' in Figure 3.20, which have the same h, k, and l Miller indices and are separated by the interplanar spacing d_{hkl}. Now assume that a parallel, monochromatic, and coherent (in-phase) beam of x-rays of wavelength λ is incident on these two planes at an angle θ. Two rays in this beam, labeled 1 and 2, are scattered by atoms P and Q. Constructive interference of the scattered rays $1'$ and $2'$ occurs also at an angle θ to the planes, 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

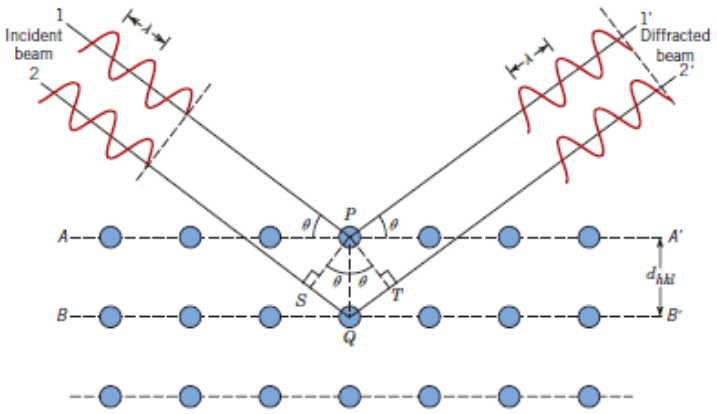


Figure 3.20 Diffraction of x-rays by planes of atoms (A–A' and B–B').

Bragg's law—relationship among x-ray wavelength, interatomic spacing, and angle of diffraction for constructive interference

$$n\lambda = \overline{SQ} + \overline{QT} \tag{3.12}$$

or

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

$$= 2d_{hkl}\sin\theta \tag{3.13}$$

Bragg's law

Equation 3.13 is known as **Bragg's law**; also, n is the order of reflection, which may be any integer (1, 2, 3, . . .) consistent with $\sin\theta$ not exceeding unity. Thus, 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.

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,

Interplanar spacing for a plane having indices h, k, and l

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \tag{3.14}$$

Example on Interplanar spacing

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. Also, assume that monochromatic radiation having a wavelength of 0.1790 nm is used, and the order of reflection is 1.

Solution

(a) The value of the interplanar spacing d_{hkl} is determined using Equation 3.14, with $a = 0.2866$ nm, and $h = 2$, $k = 2$, and $l = 0$, because we are considering the (220) planes. Therefore,

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

$$= \frac{0.2866\ \text{nm}}{\sqrt{(2)^2 + (2)^2 + (0)^2}} = 0.1013\ \text{nm}$$

(b) The value of θ may now be computed using Equation 3.13, with $n = 1$, because this is a first-order reflection:

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

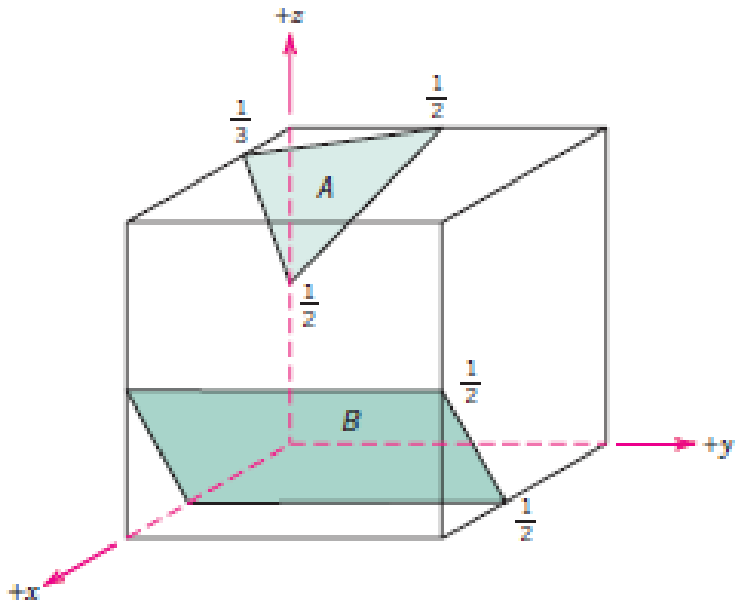
$$\theta = \sin^{-1}(0.884) = 62.13^\circ$$

The diffraction angle is 2θ, or

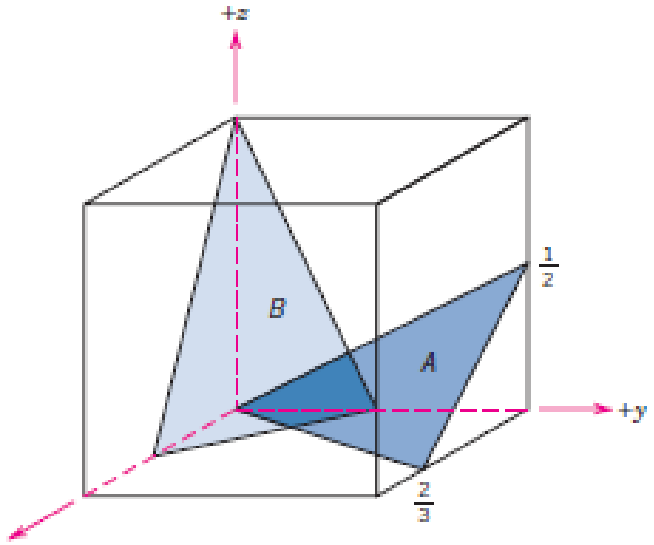
$$2\theta = (2)(62.13^\circ) = 124.26^\circ$$

Exercise Problems

Determine the Miller indices for the planes shown in the following unit cell:



Determine the Miller indices for the planes shown in the following unit cell:



Crystal X-Ray Diffraction

Figure 3.25 shows the first four peaks of the x-ray diffraction pattern for copper, which has an FCC crystal structure; monochromatic x-radiation having a wavelength of 0.1542 nm was used.

(a) Index (i.e., give h, k, and l indices for) each of these peaks.

(b) Determine the interplanar spacing for each of the peaks.

(c) For each peak, determine the atomic radius for Cu and compare these with the value presented in Table 3.1.

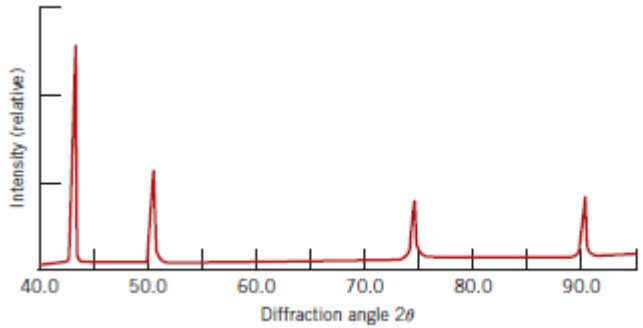


Figure 3.25 Diffraction pattern for polycrystalline copper.