3.60 How are crystallographic planes indicated in HCP unit cells?

In HCP unit cells, crystallographic planes are indicated using four indices which correspond to four axes: three basal axes of the unit cell, a_1, a_2, and a_3 , which are separated by 120º; and the vertical c axis.

3.61 What notation is used to describe HCP crystal planes?

HCP crystal planes are described using the Miller-Bravais indices, (*hkil*).

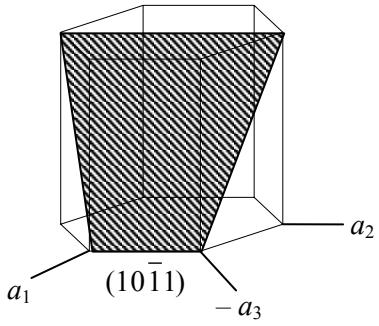
3.62 Draw the hexagonal crystal planes whose Miller-Bravais indices are:

(a) $(10\bar{1}1)$ (d) $(1\bar{2}12)$ (g) $(\bar{1}2\bar{1}2)$ (j) $(\bar{1}100)$

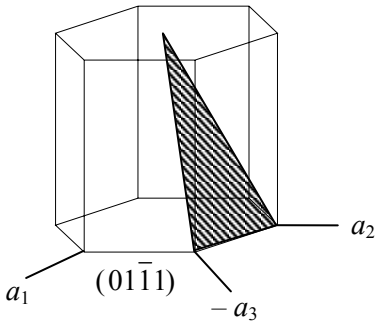
(b) $(01\bar{1}1)$ (e) $(2\bar{1}\bar{1}1)$ (h) $(2\bar{2}00)$ (k) $(\bar{2}111)$

(c) $(\bar{1}2\bar{1}0)$ (f) $(1\bar{1}01)$ (i) $(10\bar{1}2)$ (l) $(\bar{1}012)$

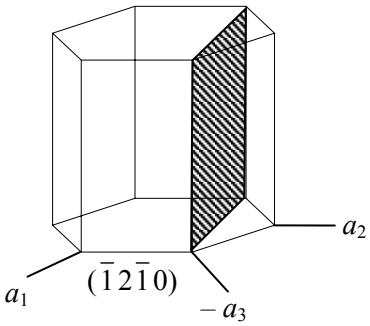
The reciprocals of the indices provided give the intercepts for the plane (a_1, a_2, a_3, and c).



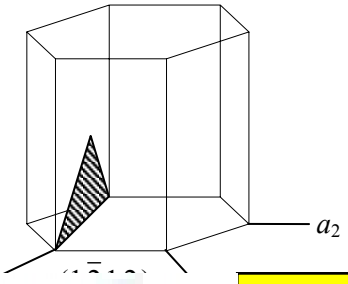
a. $a_1 = 1,\ a_2 = \infty,$
$a_3 = -1,\ c = 1$

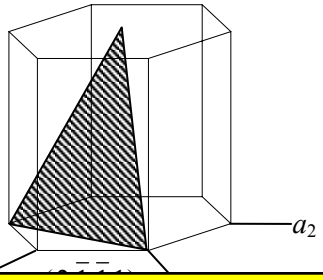


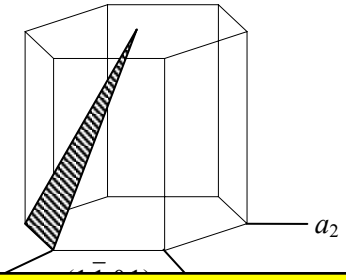
b. $a_1 = \infty,\ a_2 = 1,$
$a_3 = -1,\ c = 1$

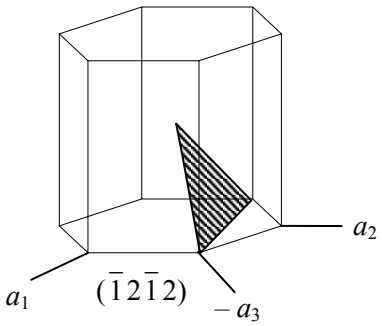


c. $a_1 = 1,\ a_2 = -\frac{1}{2},$
$a_3 = -1,\ c = \infty$

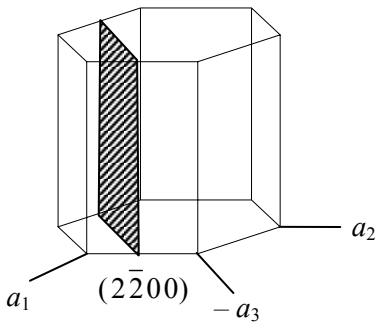




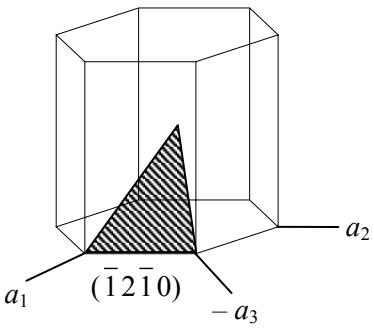




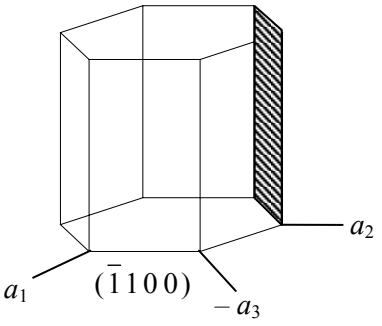
g. $a_1 = -1,\ a_2 = \frac{1}{2},$
$a_3 = -1,\ c = \frac{1}{2}$



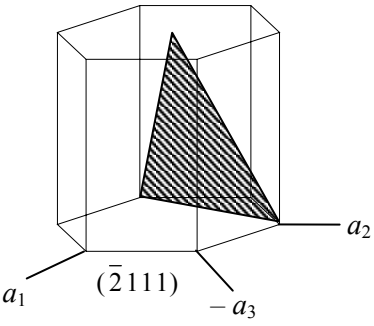
h. $a_1 = \frac{1}{2},\ a_2 = -\frac{1}{2},$
$a_3 = \infty,\ c = \infty$



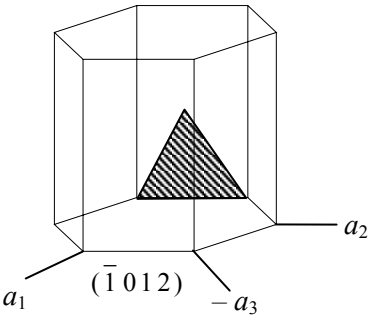
i. $a_1 = 1,\ a_2 = \infty,$
$a_3 = -1,\ c = \frac{1}{2}$



j. $a_1 = -1,\ a_2 = 1,$
$a_3 = \infty,\ c = \infty$



k. $a_1 = -\frac{1}{2},\ a_2 = 1,$
$a_3 = 1,\ c = 1$



l. $a_1 = -1,\ a_2 = \infty,$
$a_3 = 1,\ c = \frac{1}{2}$

3.63 Determine the Miller-Bravais indices of the hexagonal crystal planes in Fig. P3.63.

Miller-Bravais Indices for Planes Shown in Figure P3.63(a)

Plane *a*		**Plane *b***		**Plane *c***	
Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts
	1		1		1

Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts
$c = \infty$	$\frac{1}{c} = 0$	$c = ½$	2	$c = \infty$	$\frac{1}{c} = 0$
The Miller indices of plane *a* are **(0 $\bar{1}$ 1 0)**.		The Miller indices of plane *b* are **(1 0 $\bar{1}$ 2)**.		The Miller indices of plane *c* are **($\bar{2}$ 2 0 0)**.	

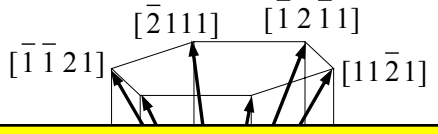
Miller-Bravais Indices for the Planes Shown in Figure P3.63(b)

Plane *a*		**Plane *b***		**Plane *c***	
Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts
$a_1 = \infty$	$\frac{1}{a_1} = 0$	$a_1 = 1$	$\frac{1}{a_1} = 1$	$a_1 = 1$	$\frac{1}{a_1} = 1$
$a_2 = 1$	$\frac{1}{a_2} = 1$	$a_2 = -1$	$\frac{1}{a_2} = -1$	$a_2 = -1$	$\frac{1}{a_2} = -1$
$a_3 = -1$	$\frac{1}{a_3} = -1$	$a_3 = \infty$	$\frac{1}{a_3} = 0$	$a_3 = \infty$	$\frac{1}{a_3} = 0$
$c = \infty$	$\frac{1}{c} = 0$	$c = 1$	$\frac{1}{c} = 1$	$c = 1$	$\frac{1}{c} = 1$
The Miller indices of plane *a* are **(0 1 $\bar{1}$ 0)**.		The Miller indices of plane *b* are **(1 $\bar{1}$ 0 1)**.		The Miller indices of plane *c* are **(1 $\bar{1}$ 0 1)**.	

3.64 Determine the Miller-Bravais direction indices of the $-a_1$, $-a_2$ and $-a_3$ directions.

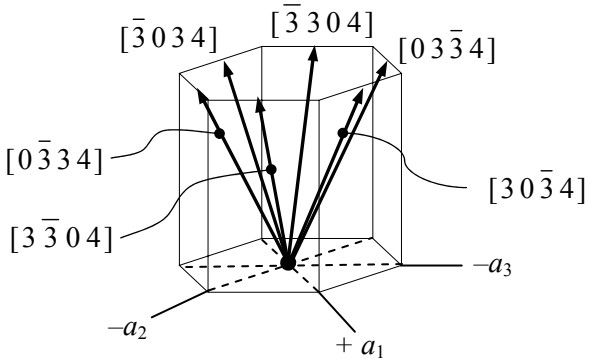
The Miller-Bravais direction indices corresponding to the $-a_1$, $-a_2$ and $-a_3$ directions are respectively, **[$\bar{1}$ 0 0 0]**, **[0 $\bar{1}$ 0 0]**, and **[0 0 $\bar{1}$ 0]**.

3.65 Determine the Miller-Bravais direction indices of the vectors originating at the center of the lower basal plane and ending at

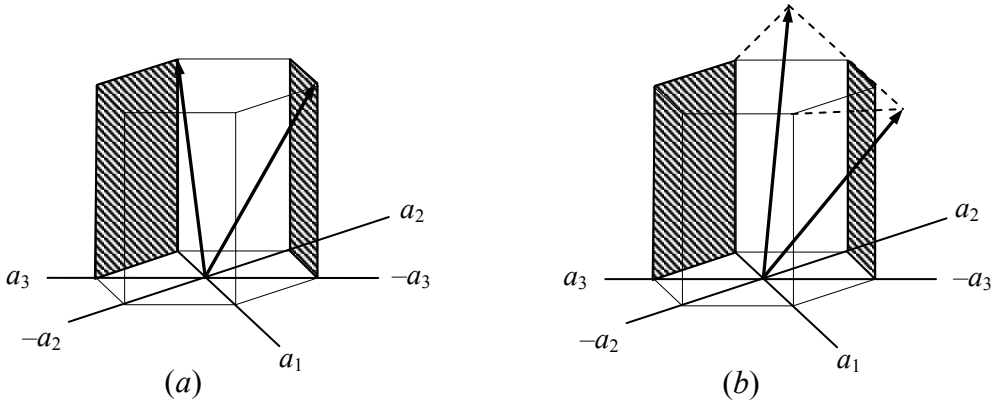


3.66 Determine the Miller-Bravais direction indices of the basal plane of the vectors originating at the center of the lower basal plane and exiting at the midpoints between the principal planar axes.

$[\bar{3}\,0\,3\,4], [\bar{3}\,3\,0\,4], [0\,3\,\bar{3}\,4],$
$[3\,0\,\bar{3}\,4], [3\,\bar{3}\,0\,4], [0\,\bar{3}\,3\,4]$



3.67 Determine the Miller-Bravais direction indices of the directions indicated in Fig. P3.67.



For Fig. P3.67(*a*), the Miller-Bravais direction indices indicated are **[$\bar{2}$ 1 1 1]** and **[1 1 $\bar{2}$ 1]**. Those associated with Fig. P3.67(*b*) are **[$\bar{1}$ 1 0 1]** and **[1 0 $\bar{1}$ 1]**.

3.68 What is the difference in the stacking arrangement of close-packed planes in (a) the HCP crystal structure and (b) the FCC crystal structure?

Although the FCC and HCP are both close-packed lattices with APF = 0.74, the structures differ in the three dimensional stacking of their planes:

(a) the stacking order of HCP planes is ABAB… ;
(b) the FCC planes have an ABCABC… stacking sequence.

3.69 What are the densest-packed planes in (a) the FCC structure and (b) the HCP structure?

(a) The most densely packed planes of the FCC lattice are the **{1 1 1}** planes.
(b) The most densely packed planes of the HCP structure are the **{0 0 0 1}** planes.

3.71 The lattice constant for BCC tantalum at 20ºC is 0.33026 nm and its density is 16.6 g/cm^3. Calculate a value for its atomic mass.

The atomic mass can be assessed based upon the mass of tantalum in a unit BCC cell:

$$\text{mass/unit cell} = \rho_v(\text{volume/unit cell}) = \rho_v a^3$$
$$= (16.6\ \text{g/cm}^3)(10^6\ \text{cm}^3/\text{m}^3)(0.33026\times10^{-9}\ \text{m})^3$$
$$= 5.98\times10^{-22}\ \text{g/u.c.}$$

Since there are two atoms in a BCC unit cell, the atomic mass is:

$$\text{Atomic mass} = \frac{(5.98\times10^{-22}\ \text{g/unit cell})(6.023\times10^{23}\ \text{atoms/mol})}{2\ \text{atoms/unit cell}}$$
$$= \mathbf{180.09\ g/mol}$$

3.72 Calculate a value for the density of FCC platinum in grams per cubic centimeter from its lattice constant *a* of 0.39239 nm and its atomic mass of 195.09 g/mol.

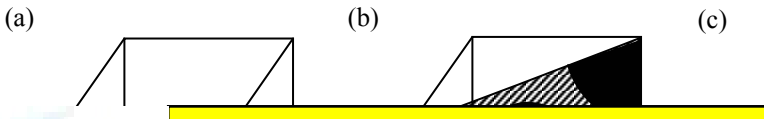
First calculate the mass per unit cell based on the atomic mass and the number of atoms per unit cell of the FCC structure,

$$\text{mass/unit cell} = \frac{(4\ \text{atoms/unit cell})(195.09\ \text{g/mol})}{6.023\times10^{23}\ \text{atoms/mol}} = 1.296\times10^{-21}\ \text{g/unit cell}$$

The density is then found as,

$$\rho_v = \frac{\text{mass/unit cell}}{\text{volume/unit cell}} = \frac{\text{mass/unit cell}}{a^3} = \frac{1.296\times10^{-21}\ \text{g/unit cell}}{[(0.39239\times10^{-9}\ \text{m})^3]/\text{unit cell}}$$
$$= 21,445,113\ \text{g/m}^3\left(\frac{\text{m}}{100\ \text{cm}}\right)^3 = \mathbf{21.45\ g/cm^3}$$

3.73 Calculate the planar atomic density in atoms per square millimeter for the following crystal planes in BCC chromium, which has a lattice constant of 0.28846 nm: (a) (100), (b) (110), (c) (111).



To calculate the density, the planar area and the number of atoms contained in that area must first be determined.

(a) The area intersected by the (1 0 0) plane inside the cubic unit cell is a^2 while the number of atoms contained is: (4 corners)× (¼ atom per corner) = 1 atom. The density is,

$$\rho_p = \frac{\text{equiv. no. of atoms whose centers are intersected by selected area}}{\text{selected area}}$$

$$= \frac{1 \text{ atom}}{(0.28846\times10^{-9} \text{ m})^2} = (1.202\times10^{19} \text{atoms/m}^2)\left(\frac{\text{m}}{1000 \text{ mm}}\right)^2$$

$$= \mathbf{1.202\times10^{13} \text{ atoms/mm}^2}$$

(b) For the more densely packed (1 1 0) plane, there are:

1 atom at center + (4 corners) × (¼ atom per corner) = 2 atoms

And the area is given as $(\sqrt{2}a)(a) = \sqrt{2}a^2$. The density is thus,

$$\rho_p = \frac{2 \text{ atoms}}{\sqrt{2}(0.28846\times10^{-9} \text{ m})^2} = (1.699\times10^{19} \text{atoms/m}^2)(10^{-6} \text{ m}^2/\text{mm}^2)$$

$$= \mathbf{1.699\times10^{13} \text{ atoms/mm}^2}$$

(c) The triangular (1 1 1) plane contains: (3 corners) × ($^1/_6$ atom per corner) = ½ atom.

The area is equal to $= \frac{1}{2}bh = \frac{1}{2}(\sqrt{2}a)\left(\frac{\sqrt{3}}{2}a\right) = \frac{\sqrt{6}}{4}a^2$. The density is thus,

$$\rho_p = \frac{1/2 \text{ atom}}{\frac{\sqrt{6}}{4}(0.28846\times10^{-9} \text{ m})^2} = (9.813\times10^{18} \text{atoms/m}^2)(10^{-6} \text{ m}^2/\text{mm}^2)$$

$$= \mathbf{9.813\times10^{12} \text{ atoms/mm}^2}$$

3.74 Calculate the planar atomic density in atoms per square millimeter for the following crystal planes in FCC gold, which has a lattice constant of 0.40788 nm: (a) (100), (b) (110), (c) (111).

(a) (b) (c)

(a) The area intersected by the (1 0 0) plane and the FCC unit cell is a^2 while the number of atoms contained is:

1 atom at center + (4 corners) × (¼ atom per corner) = 2 atoms

The density is therefore,

$$\rho_p = \frac{\text{equiv. no. of atoms whose centers are intersected by selected area}}{\text{selected area}}$$

$$= \frac{2 \text{ atoms}}{(0.40788\times10^{-9} \text{ m})^2} = (1.202\times10^{19} \text{atoms/m}^2)\left(\frac{\text{m}}{1000 \text{ mm}}\right)^2$$

$$= \mathbf{1.20\times10^{13} \text{ atoms/mm}^2}$$

(b) For the more densely packed (1 1 0) plane, there are:

(2 face atoms) × (½ atom) + (4 corners) × (¼ atom per corner) = 2 atoms

And the area is given as $(\sqrt{2}a)(a) = \sqrt{2}a^2$. The density is thus,

$$\rho_p = \frac{2 \text{ atoms}}{\sqrt{2}(0.40788\times10^{-9} \text{ m})^2} = (8.501\times10^{18} \text{atoms/m}^2)(10^{-6} \text{ m}^2/\text{mm}^2)$$

$$= \mathbf{8.50\times10^{12} \text{ atoms/mm}^2}$$

(c) The triangular (1 1 1) plane contains:

(3 face atoms × ⅓ atom) + (3 corners) × ($^1/_6$ atom per corner) = 2 atoms

The area is equal to: $= \frac{1}{2}bh = \frac{1}{2}(\sqrt{2}a)\left(\frac{\sqrt{3}}{2}a\right) = \frac{\sqrt{6}}{4}a^2$. The density is therefore,

$$\rho_p = \frac{2 \text{ atoms}}{\frac{\sqrt{6}}{4}(0.40788\times10^{-9} \text{ m})^2} = (1.963\times10^{19} \text{atoms/m}^2)(10^{-6} \text{ m}^2/\text{mm}^2)$$

$$= \mathbf{1.963\times10^{13} \text{ atoms/mm}^2}$$

3.75 Calculate the planar atomic density in atoms per

$$\text{Selected Area} = (\text{6 triangles}) \times (\text{equilateral triangle area}) = 6\left(\frac{1}{2}a\right)\left(\frac{\sqrt{3}}{2}a\right) = \frac{3\sqrt{3}}{2}a^2$$

While the number of atoms contained is:

1 atom at center + (6 corners) × (⅓ atom per corner) = 3 atoms

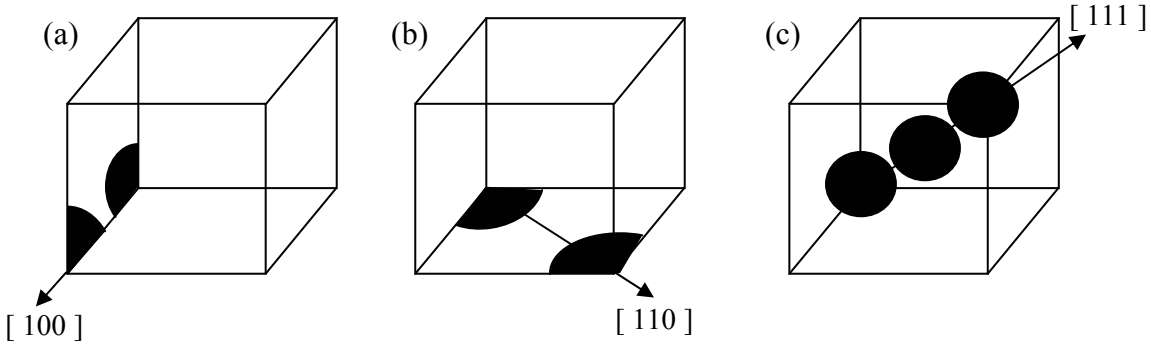
The density is therefore,

$$\rho_p = \frac{\text{equiv. no. of atoms whose centers are intersected by selected area}}{\text{selected area}}$$

$$= \frac{3 \text{ atoms}}{\frac{3\sqrt{3}}{2}(0.22856 \times 10^{-9} \text{ m})^2} = (2.201 \times 10^{19} \text{atoms/m}^2)\left(\frac{\text{m}}{1000 \text{ mm}}\right)^2$$

$$= \mathbf{2.21 \times 10^{13} \text{ atoms/mm}^2}$$

3.76 Calculate the linear atomic density in atoms per millimeter for the following directions in BCC vanadium, which has a lattice constant of 0.3039 nm:
(a) [100], (b) [110], (c) [111].



In general, the linear atomic density is derived from:

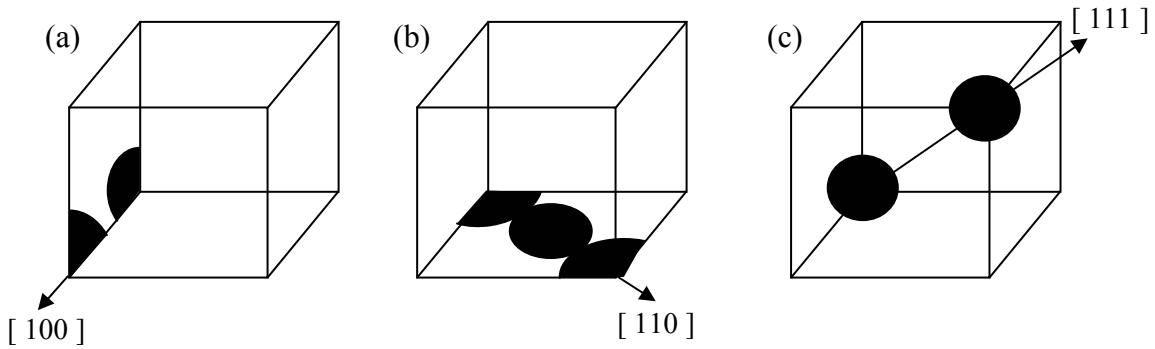
$$\rho_l = \frac{\text{no. of atomic diam. intersected by selected length of direction line}}{\text{selected length of line}}$$

$$\rho_l = \frac{\text{no. atom dia.}}{\sqrt{2}a} = \frac{1 \text{ atom}}{\sqrt{2}(0.3039 \text{ nm})(10^{-6} \text{ mm/nm})} = \mathbf{2.33 \times 10^6 \text{ mm}}$$

(c) For the [111] direction of BCC vanadium,

$$\rho_l = \frac{\text{no. atom dia.}}{\sqrt{3}a} = \frac{2 \text{ atoms}}{\sqrt{3}(0.3039 \text{ nm})(10^{-6} \text{ mm/nm})} = \mathbf{3.80 \times 10^6 \text{ mm}}$$

3.77 Calculate the linear atomic density in atoms per millimeter for the following directions in FCC iridium, which has a lattice constant of 0.38389 nm:
(a) [100], (b) [110], (c) [111].



In general, the linear atomic density is derived from:

$$\rho_l = \frac{\text{no. of atomic diam. intersected by selected length of direction line}}{\text{selected length of line}}$$

(a) For the [100] direction of FCC iridium,

$$\rho_l = \frac{\text{no. atom dia.}}{\text{a}} = \frac{1 \text{ atom}}{(0.38389 \text{ nm})(10^{-6} \text{ mm/nm})} = \mathbf{2.60 \times 10^6 \text{ mm}}$$

(b) For the [110] direction of FCC iridium,

$$\rho_l = \frac{\text{no. atom dia.}}{\sqrt{\quad}} = \frac{2 \text{ atoms}}{\sqrt{\quad}} = \mathbf{3.68 \times 10^6 \text{ mm}}$$

3.78 What is polymorphism with respect to metals?

A metal is considered polymorphic if it can exist in more than one crystalline form under different conditions of temperature and pressure.

3.79 Titanium goes through a polymorphic change from BCC to HCP crystal structure upon cooling through 882ºC. Calculate the percentage change in volume when the crystal structure changes from BCC to HCP. The lattice constant a of the BCC unit cell at 882ºC is 0.332 nm and the HCP unit cell has a = 0.2950 nm and c = 0.4683 nm.

To determine the volume change, the individual volumes per atom for the BCC and HCP structures must be calculated:

$$V_{BCC} = \frac{a^3 \text{ nm}^3/\text{unit cell}}{2 \text{ atoms/unit cell}} = \frac{(0.332 \text{ nm})^3}{2 \text{ atoms}} = 0.0183 \text{ nm}^3/\text{atom}$$

$$V_{HCP} = \frac{(3a^2c)(\sin 60^\circ) \text{ nm}^3/\text{unit cell}}{6 \text{ atoms/unit cell}} = \frac{(3)(0.2950 \text{ nm})^2(0.4683 \text{ nm})(\sin 60^\circ)}{6 \text{ atoms}}$$

$$= 0.01765 \text{ nm}^3/\text{atom}$$

Thus the change in volume due to titanium's allotropic transformation is,

$$\% \text{ Volume change} = \frac{V_{HCP} - V_{BCC}}{V_{BCC}}(100\%)$$

$$= \frac{0.01765 \text{ nm}^3/\text{atom} - 0.0183 \text{ nm}^3/\text{atom}}{0.0183 \text{ nm}^3/\text{atom}}(100\%) = \mathbf{-3.55\%}$$

3.80 Pure iron goes through a polymorphic change from BCC to FCC upon heating through 912ºC. Calculate the volume change associated with the change in crystal structure from BCC to FCC if at 912ºC the BCC unit cell has a lattice constant a = 0.293 nm and the FCC unit cell a = 0.363.

First determine the individual volumes per atom for the iron BCC and FCC crystal structures:

$$V_{BCC} = \frac{a^3 \text{ nm}^3/\text{unit cell}}{2 \text{ atoms/unit cell}} = \frac{(0.293 \text{ nm})^3}{2 \text{ atoms}} = 0.01258 \text{ nm}^3/\text{atom}$$

$$\% \text{ Volume change} = \frac{V_{FCC} - V_{BCC}}{V_{BCC}}(100\%) = \frac{0.01196 \text{ nm}^3/\text{atom} - 0.01258 \text{ nm}^3/\text{atom}}{0.01258 \text{ nm}^3/\text{atom}}(100\%)$$

$$= \mathbf{-4.94\%}$$

3.81 What are x-rays, and how are they produced?

X-rays are electromagnetic radiation having wavelengths in the range of approximately 0.05 nm to 0.25 nm. These waves are produced when accelerated electrons strike a target metal.

3.82 Draw a schematic diagram of an x-ray tube used for x-ray diffraction, and indicate on it the path of the electrons and x-rays.

See Figure 3.25 of textbook.

3.83 What is the characteristic x-ray radiation? What is its origin?

Characteristic radiation is an intense form of x-ray radiation which occurs at specific wavelengths for a particular element. The K_α radiation, the most intense characteristic radiation emitted, is caused by excited electrons dropping from the second atomic shell (n = 2) to the first shell (n = 1). The next most intense radiation, K_β, is caused by excited electrons dropping from the third atomic shell (n = 3) to the first shell (n = 1).

3.84 Distinguish between destructive interference and constructive interference of reflected x-ray beams through crystals.

Destructive interference occurs when the wave patterns of an x-ray beam, reflected from a crystal, are out of phase. Conversely, when the wave patterns leaving a crystal plane are in phase, constructive interference occurs and the beam is reinforced.

3.85 Derive Bragg's law by using the simple case of incident x-ray beams being diffracted by parallel planes in a crystal.

Referring to Fig. 3.28 (*c*), for these rays to be in phase, ray 2 must travel an additional distance of $MP + PN$. This extra length must be an integral number of wavelengths, λ.

$$n\lambda = MP + PN \text{ where } n = 1, 2, 3...$$

Moreover, the MP and PN distances must equal $d_{hkl} \sin\theta$, where d_{hkl} is the crystal

$$n\lambda = 2d_{hkl}\sin\theta \quad \text{Bragg's Law}$$

3.86 A sample of BCC metal was placed in an x-ray diffractometer using x-rays with a wavelength of λ = 0.1541 nm. Diffraction from the {221} planes was obtained at 2θ = 88.838º. Calculate a value for the lattice constant a for this BCC elemental metal (Assume first-order diffraction, n = 1.)

The interplanar distance is,

$$d_{221} = \frac{\lambda}{2\sin\theta} = \frac{0.1541\text{ nm}}{2\sin(44.419^\circ)} = 0.1101\text{ nm}$$

The lattice constant, *a*, is then,

$$a = d_{hkl}\sqrt{h^2+k^2+l^2} = (0.1101\text{ nm})\sqrt{2^2+2^2+1^2} = \mathbf{0.3303\ nm}$$

3.87 X-rays of an unknown wavelength are diffracted by a gold sample. The 2θ angle was 64.582º for the {220} planes. What is the wavelength of the x-rays used? (The lattice constant of gold is 0.40788 nm. Assume first-order diffraction, n = 1.)

The interplanar distance is,

$$d_{220} = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{0.40788\text{ nm}}{\sqrt{2^2+2^2+0^2}} = \mathbf{0.1442\ nm}$$

The lattice constant, *a*, is then,

$$\lambda = 2d_{221}\sin\theta = 2(0.1442\text{ nm})\sin(32.291^\circ) = \mathbf{0.154\ nm}$$

3.88 An x-ray diffractometer recorder chart for an element which has either the BCC or the FCC crystal structure showed diffraction peaks at the following 2θ angles: 41.069º, 47.782º, 69.879º, and 84.396º. (The wavelength of the incoming radiation was 0.15405 nm.)
(a) Determine the crystal structure of the element.
(b) Determine the lattice constant of the element.
(c) Identify the element.

$$\frac{\sin^2\theta_1}{\sin^2\theta_2} = \frac{0.12304}{0.16402} = \mathbf{0.75} \Rightarrow \mathbf{FCC}$$

(b) The lattice constant also depends upon the first $\sin^2\theta$ term, as well as, the Miller indices of the first set of FCC principal diffracting planes, {111}.

$$a = \frac{\lambda}{2}\sqrt{\frac{h^2+k^2+l^2}{\sin^2\theta_1}} = \frac{0.15405\text{ nm}}{2}\sqrt{\frac{1^2+1^2+1^2}{0.12304}} = \mathbf{0.38034\text{ nm}}$$

(c) From Appendix I, the FCC metal whose lattice constant is closest to 0.38034 nm is **rhodium (Rh)** which has a lattice constant of 0.38044 nm.

3.89 An x-ray diffractometer recorder chart for an element which has either the BCC or the FCC crystal structure showed diffraction peaks at the following 2θ angles: 38.60º, 55.71º, 69.70º, 82.55º, 95.00º, and 107.67º. (The wavelength λ of the incoming radiation was 0.15405 nm.)
(a) Determine the crystal structure of the element.
(b) Determine the lattice constant of the element.
(c) Identify the element.

(a) Comparing the $\sin^2\theta$ term for the first two angles:

2θ	θ	$\sin\theta$	$\sin^2\theta$
38.60°	19.30°	0.33051	0.10924
55.71°	27.855°	0.46724	0.21831

$$\frac{\sin^2\theta_1}{\sin^2\theta_2} = \frac{0.10924}{0.21831} = \mathbf{0.50} \Rightarrow \mathbf{BCC}$$

(b) The lattice constant also depends upon the first $\sin^2\theta$ term, as well as, the Miller indices of the first set of BCC principal diffracting planes {110}.

$$a = \frac{\lambda}{2}\sqrt{\frac{h^2+k^2+l^2}{\sin^2\theta_1}} = \frac{0.15405\text{ nm}}{2}\sqrt{\frac{1^2+1^2+0^2}{0.10924}} = \mathbf{0.3296\text{ nm}}$$

3.90 An x-ray diffractometer recorder chart for an element which has either the BCC or the FCC crystal structure showed diffraction peaks at the following 2θ angles: 36.191º, 51.974º, 64.982º, and 76.663º. (The wavelength λ of the incoming radiation was 0.15405 nm.)

(a) Determine the crystal structure of the element.
(b) Determine the lattice constant of the element.
(c) Identify the element.

(a) Comparing the $\sin^2\theta$ term for the first two angles:

2θ	θ	$\sin\theta$	$\sin^2\theta$
36.191°	18.096°	0.31060	0.09647
51.974°	25.987°	0.43817	0.19199

$$\frac{\sin^2\theta_1}{\sin^2\theta_2} = \frac{0.09647}{0.19199} = \mathbf{0.50} \Rightarrow \mathbf{BCC}$$

(b) The lattice constant also depends upon the first $\sin^2\theta$ term, as well as, the Miller indices of the first set of BCC principal diffracting planes, {110}.

$$a = \frac{\lambda}{2}\sqrt{\frac{h^2+k^2+l^2}{\sin^2\theta_1}} = \frac{0.15405\text{ nm}}{2}\sqrt{\frac{1^2+1^2+0^2}{0.09647}} = \mathbf{0.35071\,nm}$$

(c) From Appendix I, the BCC metal whose lattice constant is closest to 0.35071 nm is **lithium (Li)** which has a lattice constant of 0.35092 nm.

3.91 An x-ray diffractometer recorder chart for an element which has either the BCC or the FCC crystal structure showed diffraction peaks at the following 2θ angles: 40.663º, 47.314º, 69.144º, and 83.448º. (The wavelength λ of the incoming radiation was 0.15405 nm.)

(a) Determine the crystal structure of the element.
(b) Determine the lattice constant of the element.
(c) Identify the element.

(a) Comparing the $\sin^2\theta$ term for the first two angles:

$$\frac{\sin^2\theta_1}{\sin^2\theta_2} = \frac{0.12072}{0.16101} = \mathbf{0.75} \Rightarrow \mathbf{FCC}$$

(b) The lattice constant also depends upon the first $\sin^2\theta$ term, as well as, the Miller indices of the first set of FCC principal diffracting planes, {111}.

$$a = \frac{\lambda}{2}\sqrt{\frac{h^2+k^2+l^2}{\sin^2\theta_1}} = \frac{0.15405 \text{ nm}}{2}\sqrt{\frac{1^2+1^2+1^2}{0.12072}} = \mathbf{0.38397 \text{ nm}}$$

(c) From Appendix I, the FCC metal whose lattice constant is closest to 0.38397 nm is **iridium (Ir)** which has a lattice constant of 0.38389 nm.