

CHAPTER 3 ATOMIC STRUCTURE AND BONDING

- 3.1 Define a crystalline solid.

A crystalline solid is one which has a crystal structure in which atoms or ions are arranged in a pattern that repeats itself in three dimensions.

- 3.2 Define a crystal structure. Give examples of materials which have crystal structures.

A crystal structure is identical to a crystalline solid, as defined by the solution of Problem 3.1. Examples include metals, ionic crystals and certain ceramic materials.

- 3.3 Define a space lattice.

A space lattice is an infinite three-dimensional array of points with each point having identical surrounding points.

- 3.4 Define a unit cell of a space lattice. What lattice constants define a unit cell?

The unit cell of a space lattice represents a repeating unit of atomic spatial positions. The cell is defined by the magnitudes and directions of three lattice vectors, **a**, **b**, and **c**: axial lengths *a*, *b*, and *c*; interaxial angles α , β , and γ .

- 3.5 What are the 14 Bravais unit cells?

The fourteen Bravais lattices are: simple cubic, body-centered cubic, face-centered cubic, simple tetragonal, body-centered tetragonal, simple orthorhombic, base-centered orthorhombic, body-centered orthorhombic, face-centered orthorhombic, simple rhombohedral, simple hexagonal, simple monoclinic, base-centered monoclinic, and simple triclinic.

- 3.6 What are the three most common metal crystal structures? List five metals which have each of these crystal structures.

The three most common crystal structures found in metals are: body-centered cubic (BCC), face-centered cubic (FCC), and hexagonal close-packed (HCP). Examples of

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A BCC crystal structure has **two** atoms in each unit cell.

- 3.8 What is the coordination number for the atoms in the BCC crystal structure?

A BCC crystal structure has a coordination number of **eight**.

- 3.9 What is the relationship between the length of the side a of the BCC unit cell and the radius of its atoms?

In a BCC unit cell, one complete atom and two atom eighths touch each other along the cube diagonal. This geometry translates into the relationship $\sqrt{3}a = 4R$.

- 3.10 Molybdenum at 20°C is BCC and has an atomic radius of 0.140 nm. Calculate a value for its lattice constant a in nanometers.

Letting a represent the edge length of the BCC unit cell and R the molybdenum atomic radius,

$$\sqrt{3}a = 4R \quad \text{or} \quad a = \frac{4}{\sqrt{3}}R = \frac{4}{\sqrt{3}}(0.140 \text{ nm}) = \mathbf{0.323 \text{ nm}}$$

- 3.11 Niobium at 20°C is BCC and has an atomic radius of 0.143 nm. Calculate a value for its lattice constant a in nanometers.

For a BCC unit cell having an edge length a and containing niobium atoms,

$$\sqrt{3}a = 4R \quad \text{or} \quad a = \frac{4}{\sqrt{3}}R = \frac{4}{\sqrt{3}}(0.143 \text{ nm}) = \mathbf{0.330 \text{ nm}}$$

- 3.12 Lithium at 20°C is BCC and has an atomic radius of 0.35092 nm. Calculate a value for the atomic radius of a lithium atom in nanometers.

For the lithium BCC structure, which has a lattice constant of $a = 0.35092 \text{ nm}$, the atomic radius is,

$$R = \frac{\sqrt{3}}{4}a = \frac{\sqrt{3}}{4}(0.35092 \text{ nm}) = \mathbf{0.152 \text{ nm}}$$

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$$R = \frac{\sqrt{3}}{4} a = \frac{\sqrt{3}}{4} (0.42906 \text{ nm}) = \mathbf{0.186 \text{ nm}}$$

- 3.14 How many atoms per unit cell are there in the FCC crystal structure?

Each unit cell of the FCC crystal structure contains **four** atoms.

- 3.15 What is the coordination number for the atoms in the FCC crystal structure?

The FCC crystal structure has a coordination number of **twelve**.

- 3.16 Gold is FCC and has a lattice constant of 0.40788 nm. Calculate a value for the atomic radius of a gold atom in nanometers.

For the gold FCC structure, which has a lattice constant of $a = 0.40788 \text{ nm}$, the atomic radius is,

$$R = \frac{\sqrt{2}}{4} a = \frac{\sqrt{2}}{4} (0.40788 \text{ nm}) = \mathbf{0.144 \text{ nm}}$$

- 3.17 Platinum is FCC and has a lattice constant of 0.39239 nm. Calculate a value for the atomic radius of a platinum atom in nanometers.

For the platinum FCC structure, with a lattice constant of $a = 0.39239 \text{ nm}$, the atomic radius is,

$$R = \frac{\sqrt{2}}{4} a = \frac{\sqrt{2}}{4} (0.39239 \text{ nm}) = \mathbf{0.139 \text{ nm}}$$

- 3.18 Palladium is FCC and has an atomic radius of 0.137 nm. Calculate a value for its lattice constant a in nanometers.

Letting a represent the FCC unit cell edge length and R the palladium atomic radius,

$$\sqrt{2}a = 4R \quad \text{or} \quad a = \frac{4}{\sqrt{2}} R = \frac{4}{\sqrt{2}} (0.137 \text{ nm}) = \mathbf{0.387 \text{ nm}}$$

- 3.19 Strontium is FCC and has an atomic radius of 0.215 nm. Calculate a value for its lattice

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- 3.20 Calculate the atomic packing factor for the FCC structure.

By definition, the atomic packing factor is given as:

$$\text{Atomic packing factor} = \frac{\text{volume of atoms in FCC unit cell}}{\text{volume of the FCC unit cell}}$$

These volumes, associated with the four-atom FCC unit cell, are

$$V_{\text{atoms}} = 4 \left[\frac{4}{3} \pi R^3 \right] = \frac{16}{3} \pi R^3 \quad \text{and} \quad V_{\text{unit cell}} = a^3$$

where a represents the lattice constant. Substituting $a = \frac{4R}{\sqrt{2}}$,

$$V_{\text{unit cell}} = a^3 = \frac{64R^3}{2\sqrt{2}}$$

The atomic packing factor then becomes,

$$\text{APF (FCC unit cell)} = \left(\frac{16\pi R^3}{3} \right) \left(\frac{1\sqrt{2}}{32R^3} \right) = \frac{\pi\sqrt{2}}{6} = 0.74$$

- 3.21 How many atoms per unit cell are there in the HCP crystal structure?

The hexagonal prism contains **six** atoms.

- 3.22 What is the coordination number for the atoms in the HCP crystal structure?

The coordination number associated with the HCP crystal structure is **twelve**.

- 3.23 What is the ideal c/a ratio for HCP metals?

The ideal c/a ratio for HCP metals is **1.633**; however, the actual ratios may deviate significantly from this value.

- 3.24 Of the following HCP metals, which have higher or lower c/a ratios than the ideal ratio:
Zr, Ti, Zn, Mg, Co, Cd and Be?



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$$\begin{aligned}
 V &= (\text{Area of Base})(\text{Height}) = [(6 \times \text{Equilateral Triangle Area})(\text{Height})] \\
 &= (3a^2 \sin 60^\circ)(c) \\
 &= 3(0.29504 \text{ nm})^2 (\sin 60^\circ)(0.46833 \text{ nm}) \\
 &= \mathbf{0.106 \text{ nm}^3}
 \end{aligned}$$

- 3.26 Rhenium at 20°C is HCP. The height c of its unit cell is 0.44583 nm and its c/a ratio is 1.633 nm. Calculate a value for its lattice constant a in nanometers.

The rhenium lattice constant a is calculated as,

$$a = \frac{c}{c/a} = \frac{0.44583 \text{ nm}}{1.633} = \mathbf{0.273 \text{ nm}}$$

- 3.27 Osmium at 20°C is HCP. Using a value of 0.135 nm for the atomic radius of osmium atoms, calculate a value for its unit-cell volume. Assume a packing factor of 0.74.

From the definition of the atomic packing factor,

$$\text{HCP unit cell volume} = \frac{\text{volume of atoms in HCP unit cell}}{\text{APF}}$$

Since there are six atoms in the HCP unit cell, the volume of atoms is:

$$V_{\text{atoms}} = 6 \left(\frac{4}{3} \pi R^3 \right) = 8\pi(0.135)^3 = 0.0618 \text{ nm}^3$$

The unit cell volume thus becomes,

$$\text{HCP unit cell volume} = \frac{0.0618 \text{ nm}^3}{0.74} = \mathbf{0.084 \text{ nm}^3}$$

- 3.28 How are atomic positions located in cubic unit cells?

Atomic positions are located in cubic unit cells using rectangular x , y , and z axes and unit distances along the respective axes. The directions of these axes are shown below.



+z
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- 3.29 List the atom positions for the eight corner and six face-centered atoms of the FCC unit cell.

The atom positions at the corners of an FCC unit cell are:

$(0, 0, 0), (1, 0, 0), (-1, 1, 0), (0, 1, 0), (0, 0, 1), (1, 0, 1), (1, 1, 1), (0, 1, 1)$

On the faces of the FCC unit cell, atoms are located at:

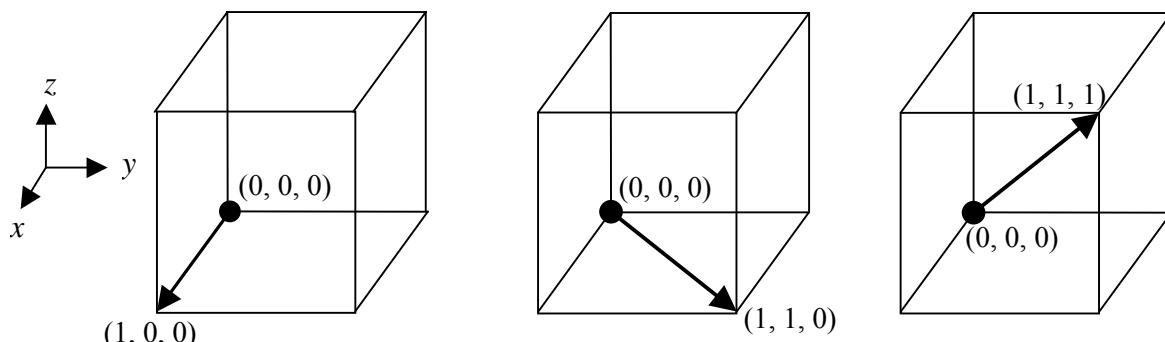
$(\frac{1}{2}, \frac{1}{2}, 0), (\frac{1}{2}, 0, \frac{1}{2}), (0, \frac{1}{2}, \frac{1}{2}), (\frac{1}{2}, \frac{1}{2}, 1), (1, \frac{1}{2}, \frac{1}{2}), (\frac{1}{2}, 1, \frac{1}{2})$

- 3.30 How are the indices for a crystallographic direction in a cubic unit cell determined?

For cubic crystals, the crystallographic direction indices are the components of the direction vector, resolved along each of the coordinate axes and reduced to the smallest integers. These indices are designated as $[uvw]$.

- 3.31 Draw the following directions in a BCC unit cell and list the position coordinates of the atoms whose centers are intersected by the direction vector:

(a) $[100]$ (b) $[110]$ (c) $[111]$



(a) Position Coordinates: $(0, 0, 0), (1, 0, 0)$ (b) Position Coordinates: $(0, 0, 0), (1, 1, 0)$ (c) Position Coordinates: $(0, 0, 0), (1, 1, 1)$

- 3.32 Draw direction vectors in unit cubes for the following cubic directions:

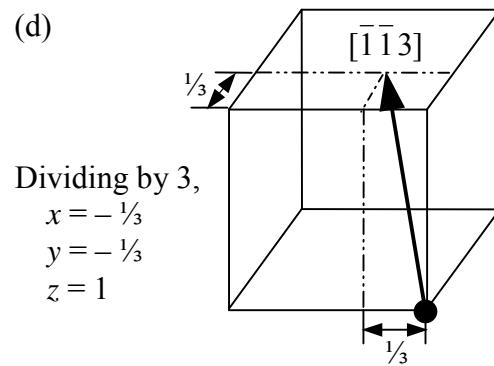
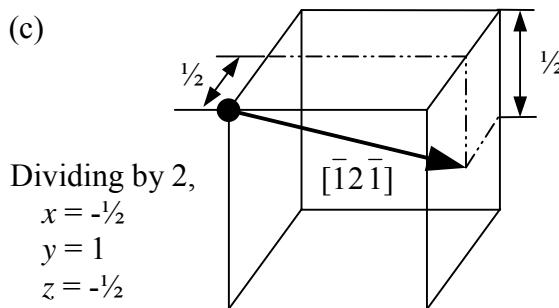
(a) $[1\bar{1}\bar{1}]$ (b) $[1\bar{1}0]$ (c) $[\bar{1}2\bar{1}]$ (d) $[\bar{1}\bar{1}3]$

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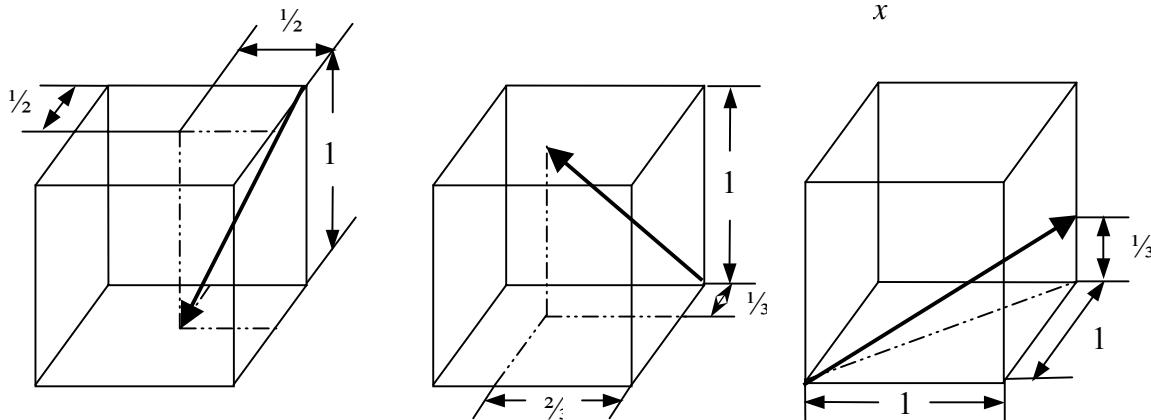
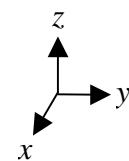
$[1\bar{1}\bar{1}]$

$[1\bar{1}0]$



3.33 Draw direction vectors in unit cubes for the following cubic directions:

- (a) $[1\bar{1}\bar{2}]$
- (d) $[0\bar{2}1]$
- (g) $[\bar{1}01]$
- (j) $[10\bar{3}]$
- (b) $[1\bar{2}3]$
- (e) $[2\bar{1}2]$
- (h) $[12\bar{1}]$
- (k) $[1\bar{2}\bar{2}]$
- (c) $[\bar{3}31]$
- (f) $[2\bar{3}3]$
- (i) $[321]$
- (l) $[\bar{2}\bar{2}3]$



(a) Dividing $[1\bar{1}\bar{2}]$ by 2,

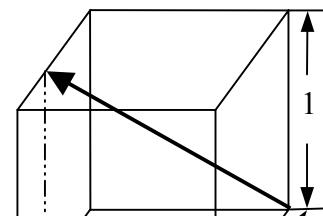
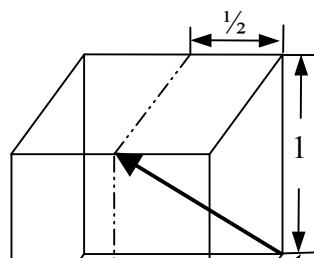
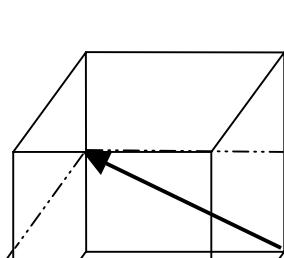
$$x = \frac{1}{2}, y = -\frac{1}{2}, z = -1$$

(b) Dividing $[12\bar{3}]$ by 3,

$$x = \frac{1}{3}, y = -\frac{2}{3}, z = 1$$

(c) Dividing $[\bar{3}31]$ by 3,

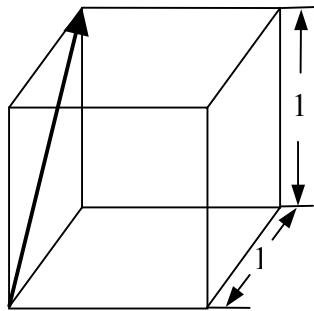
$$x = -1, y = 1, z = \frac{1}{3}$$



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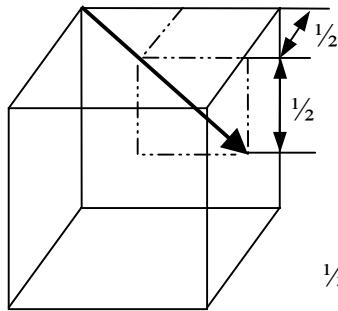
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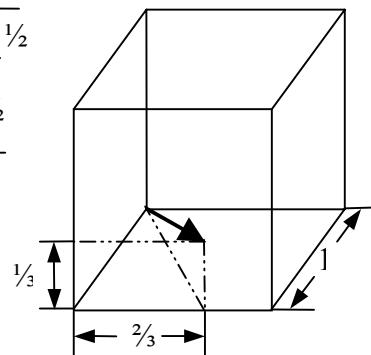
(g) For $\bar{[1}01]$,

$$x = -1, y = 0, z = 1$$



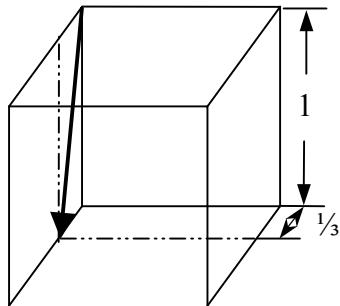
(h) Dividing $[12\bar{1}]$ by 2,

$$x = \frac{1}{2}, y = 1, z = -\frac{1}{2}$$



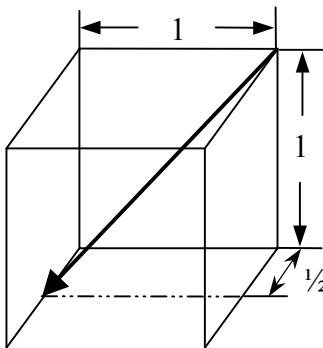
(i) Dividing $[321]$ by 3,

$$x = 1, y = \frac{2}{3}, z = \frac{1}{3}$$



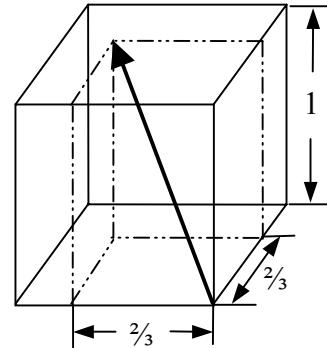
(j) Dividing $[10\bar{3}]$ by 3,

$$x = \frac{1}{3}, y = 0, z = -1$$



(k) Dividing $[1\bar{2}\bar{2}]$ by 2,

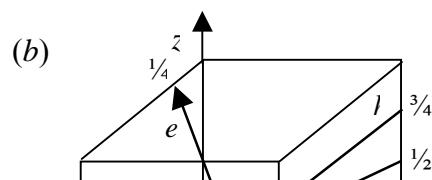
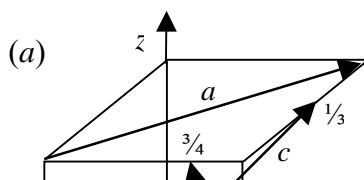
$$x = \frac{1}{2}, y = -1, z = -1$$



(l) Dividing $[\bar{2}\bar{2}3]$ by 3,

$$x = -\frac{2}{3}, y = -\frac{2}{3}, z = 1$$

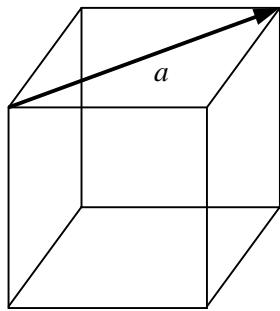
3.34 What are the indices of the directions shown in the unit cubes of Fig. P3.34?



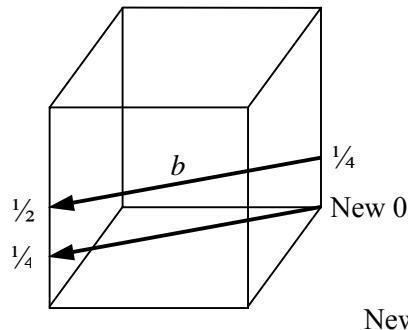
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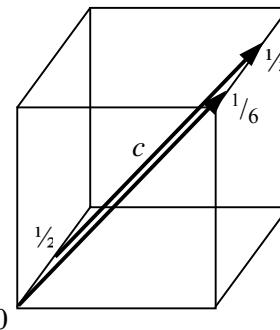
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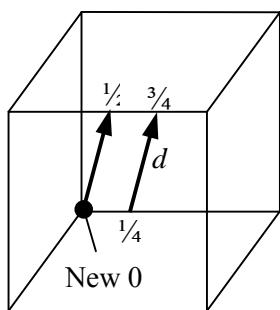
- a. Vector components:
 $x = -1, y = 1, z = 0$
 Direction indices: $[1\bar{1}0]$



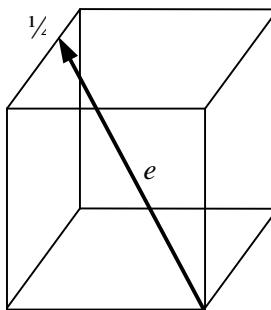
- b. Moving direction vector down $\frac{1}{4}$, vector components are: $x = 1, y = -1, z = \frac{1}{4}$
 Direction indices: $[4\bar{4}1]$



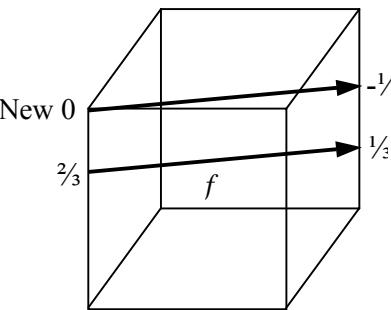
- c. Moving direction vector forward $\frac{1}{2}$, vector components are: $x = -\frac{1}{6}, y = 1, z = 1$
 Direction indices: $[1\bar{6}\bar{6}]$



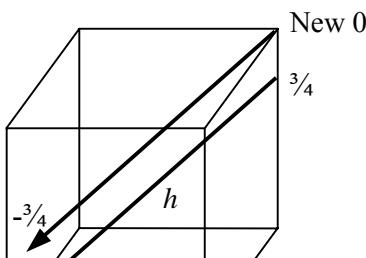
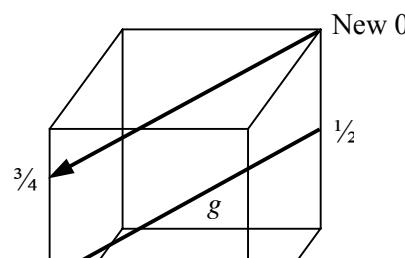
- d. Moving direction vector left $\frac{1}{4}$, vector components are: $x = 1, y = \frac{1}{2}, z = 1$
 Direction indices: $[212]$



- e. Vector components are:
 $x = -\frac{3}{4}, y = -1, z = 1$
 Direction indices: $[3\bar{4}\bar{4}]$



- f. Moving direction vector up $\frac{1}{3}$, vector components are:
 $x = -1, y = 1, z = -\frac{1}{3}$
 Direction indices: $[3\bar{3}\bar{1}]$



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- 3.35 A direction vector passes through a unit cube from the ($\frac{3}{4}$, 0, $\frac{1}{4}$) to the ($\frac{1}{2}$, 1, 0) positions. What are its direction indices?

The starting point coordinates, subtracted from the end point, give the vector components:

$$x = \frac{1}{2} - \frac{3}{4} = -\frac{1}{4} \quad y = 1 - 0 = 1 \quad z = 0 - \frac{1}{4} = -\frac{1}{4}$$

The fractions can then be cleared through multiplication by 4, giving $x = -1$, $y = 4$, $z = -1$. The direction indices are therefore [$\bar{1} \ 4 \ \bar{1}$].

- 3.36 A direction vector passes through a unit cube from the (1, 0, $\frac{3}{4}$) to the ($\frac{1}{4}$, 1, $\frac{1}{4}$) positions. What are its direction indices?

Subtracting coordinates, the vector components are:

$$x = \frac{1}{4} - 1 = -\frac{3}{4} \quad y = 1 - 0 = 1 \quad z = \frac{1}{4} - \frac{3}{4} = -\frac{1}{2}$$

Clearing fractions through multiplication by 4, gives $x = -3$, $y = 4$, $z = -2$. The direction indices are therefore [$\bar{3} \ 4 \ \bar{2}$].

- 3.37 What are the crystallographic directions of a family or form? What generalized notation is used to indicate them?

A family or form has equivalent crystallographic directions; the atom spacing along each direction is identical. These directions are indicated by $\langle uvw \rangle$.

- 3.38 What are the directions of the $\langle 100 \rangle$ family or form for a unit cube?

$$[100], [010], [001], [\bar{1}00], [0\bar{1}0], [00\bar{1}]$$

- 3.39 What are the directions of the $\langle 111 \rangle$ family or form for a unit cube?

$$\begin{aligned} &[111], [\bar{1}\bar{1}\bar{1}], [\bar{1}\bar{1}1], [\bar{1}1\bar{1}], \\ &[\bar{1}11], [1\bar{1}\bar{1}], [1\bar{1}1], [\bar{1}\bar{1}1] \end{aligned} \quad \begin{matrix} [1\bar{1}1] \\ [11\bar{1}] \\ [1\bar{1}\bar{1}] \end{matrix} \quad [0\bar{1}1]$$

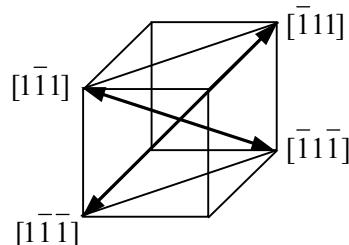
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- 3.41 What $\langle 111 \rangle$ -type directions lie on the (110) plane of a cubic unit cell?

[1 $\bar{1}$ 1], [11 $\bar{1}$], [1 $\bar{1}$ $\bar{1}$], [$\bar{1}$ 11]

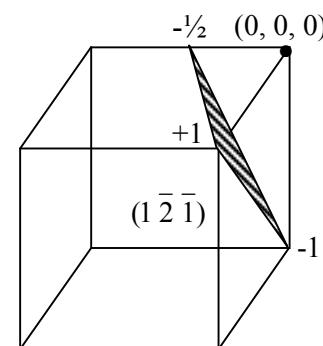
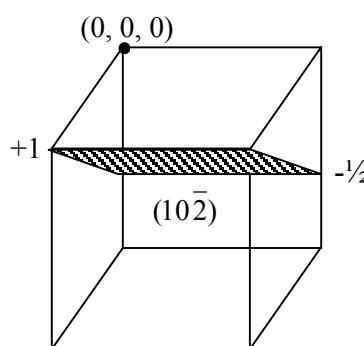
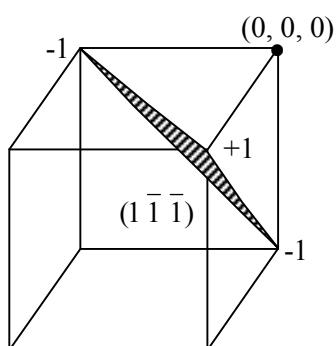
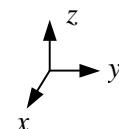


- 3.42 How are the Miller indices for a crystallographic plane in a cubic unit cell determined? What generalized notation is used to indicate them?

The Miller indices are determined by first identifying the fractional intercepts which the plane makes with the crystallographic x , y , and z axes of the cubic unit cell. Then all fractions must be cleared such that the smallest set of whole numbers is attained. The general notation used to indicate these indices is (hkl) , where h , k , and l correspond to the x , y and z axes, respectively.

- 3.43 Draw in unit cubes the crystal planes that have the following Miller indices:

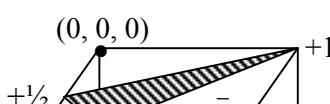
- (a) (1 $\bar{1}\bar{1}$) (d) (21 $\bar{3}$) (g) (20 $\bar{1}$) (j) (13 $\bar{3}$)
 (b) (10 $\bar{2}$) (e) (3 $\bar{2}$ 1) (h) ($\bar{2}$ 1 $\bar{2}$) (k) (3 $\bar{1}$ 2)
 (c) (1 $\bar{2}\bar{1}$) (f) (30 $\bar{2}$) (i) ($\bar{2}$ 32) (l) ($\bar{3}$ 3 $\bar{1}$)



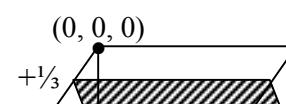
a. For (1 $\bar{1}\bar{1}$) reciprocals
are: $x = 1$, $y = -1$, $z = -1$

b. For (10 $\bar{2}$) reciprocals
are: $x = 1$, $y = \infty$, $z = -\frac{1}{2}$

c. For (1 $\bar{2}\bar{1}$) reciprocals
are: $x = 1$, $y = -\frac{1}{2}$, $z = -1$



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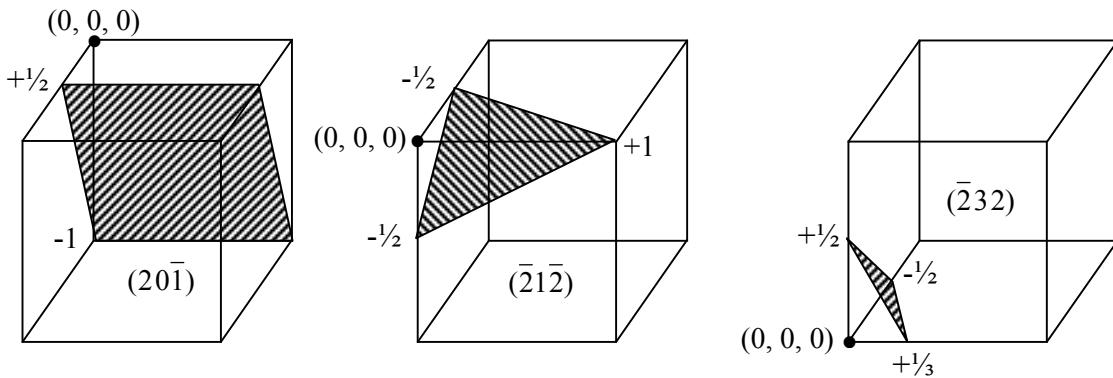
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are: $x = \frac{1}{2}$, $y = 1$, $z = -\frac{1}{3}$ are: $x = \frac{1}{3}$, $y = -\frac{1}{2}$, $z = 1$ are: $x = \frac{1}{3}$, $y = \infty$, $z = -\frac{1}{2}$

Smith Foundations of Materials Science and Engineering Solution Manual 31

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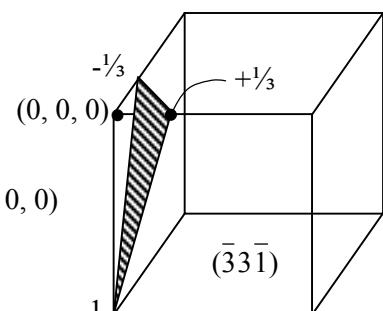
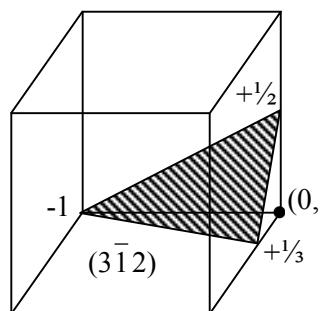
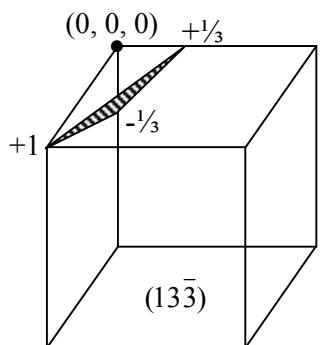
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g. For $(20\bar{1})$ reciprocals
are: $x = \frac{1}{2}$, $y = \infty$, $z = -1$

h. For $(\bar{2}1\bar{2})$ reciprocals
are: $x = -\frac{1}{2}$, $y = 1$, $z = -\frac{1}{2}$

i. For $(\bar{2}32)$ reciprocals are:
 $x = -\frac{1}{2}$, $y = \frac{1}{3}$, $z = \frac{1}{2}$

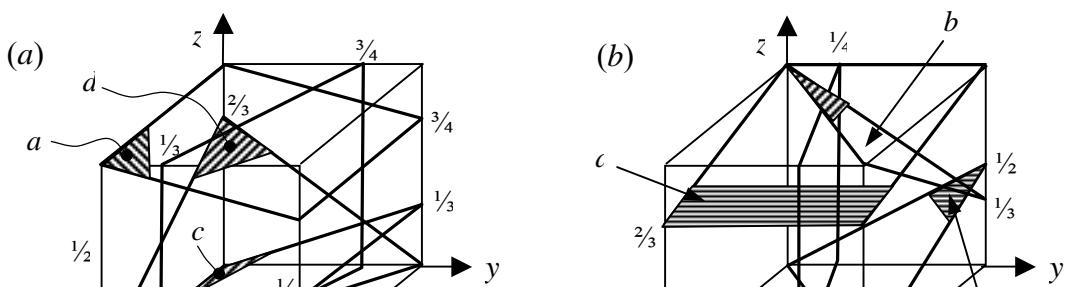


j. For $(13\bar{3})$ reciprocals
are: $x = 1$, $y = \frac{1}{3}$, $z = -\frac{1}{3}$

k. For $(3\bar{1}2)$ reciprocals
are: $x = \frac{1}{3}$, $y = -1$, $z = \frac{1}{2}$

k. For $(\bar{3}3\bar{1})$ reciprocals
are: $x = -\frac{1}{3}$, $y = \frac{1}{3}$, $z = -1$

3.44 What are the Miller indices of the cubic crystallographic planes shown in Fig. P3.44?



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Miller Indices for Figure P3.44(a)

Plane <i>a</i> based on (0, 1, 1) as origin		Plane <i>b</i> based on (1, 1, 0) as origin	
Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts
$x = \infty$	$\frac{1}{x} = 0$	$x = -1$	$\frac{1}{x} = -1$
$y = -1$	$\frac{1}{y} = -1$	$y = \frac{-5}{12}$	$\frac{1}{y} = \frac{-12}{5}$
$z = -\frac{1}{4}$	$\frac{1}{z} = -4$	$z = \infty$	$\frac{1}{z} = 0$

The Miller indices of plane *a* are $(0\bar{1}\bar{4})$. The Miller indices of plane *b* are $(\bar{5}\bar{1}\bar{2}0)$.

Plane <i>c</i> based on (1, 1, 0) as origin		Plane <i>d</i> based on (0, 0, 0) as origin	
Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts
$x = \infty$	$\frac{1}{x} = 0$	$x = 1$	$\frac{1}{x} = 1$
$y = -1$	$\frac{1}{y} = -1$	$y = 1$	$\frac{1}{y} = 1$
$z = \frac{1}{3}$	$\frac{1}{z} = 3$	$z = \frac{2}{3}$	$\frac{1}{z} = \frac{3}{2}$

The Miller indices of plane *c* are $(0\bar{1}3)$. The Miller indices of plane *d* are $(2\bar{2}3)$.

Miller Indices for Figure P3.44(b)

Plane <i>a</i> based on (1, 0, 1) as origin		Plane <i>b</i> based on (0, 1, 1) as origin	
Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts
$x = -1$	$\frac{1}{x} = -1$	$x = 1$	$\frac{1}{x} = 1$

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Plane <i>c</i> based on (0, 1, 0) as origin		Plane <i>d</i> based on (0, 1, 0) as origin	
Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts
$x = 1$	$\frac{1}{x} = 1$	$x = 1$	$\frac{1}{x} = 1$
$y = \frac{-5}{12}$	$\frac{1}{y} = \frac{-12}{5}$	$y = -1$	$\frac{1}{y} = -1$
$z = \infty$	$\frac{1}{z} = 0$	$z = \frac{1}{2}$	$\frac{1}{z} = 2$
The Miller indices of plane <i>c</i> are (5 12 0).		The Miller indices of plane <i>d</i> are (1 12).	

- 3.45 What is the notation used to indicate a family or form of cubic crystallographic planes?

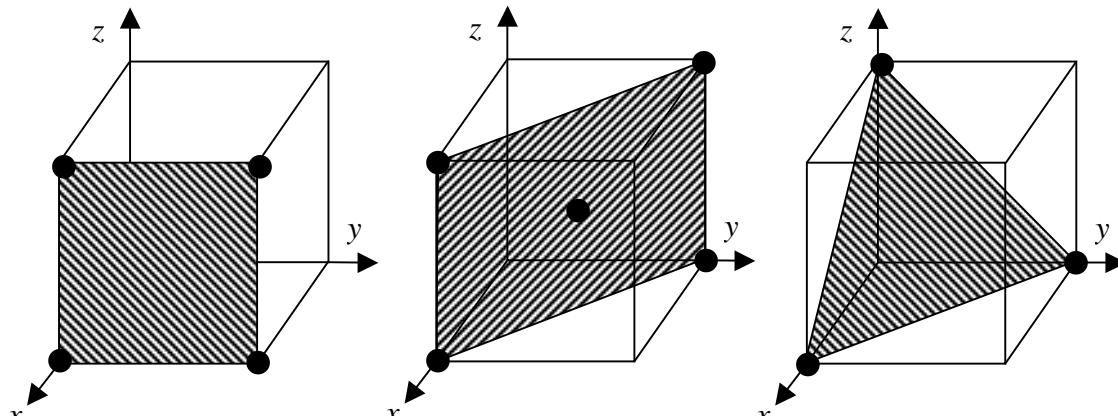
A family or form of a cubic crystallographic plane is indicated using the notation $\{hkl\}$.

- 3.46 What are the {100} family of planes of the cubic system?

$$(100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1})$$

- 3.47 Draw the following crystallographic planes in a BCC unit cell and list the position of the atoms whose centers are intersected by each of the planes:

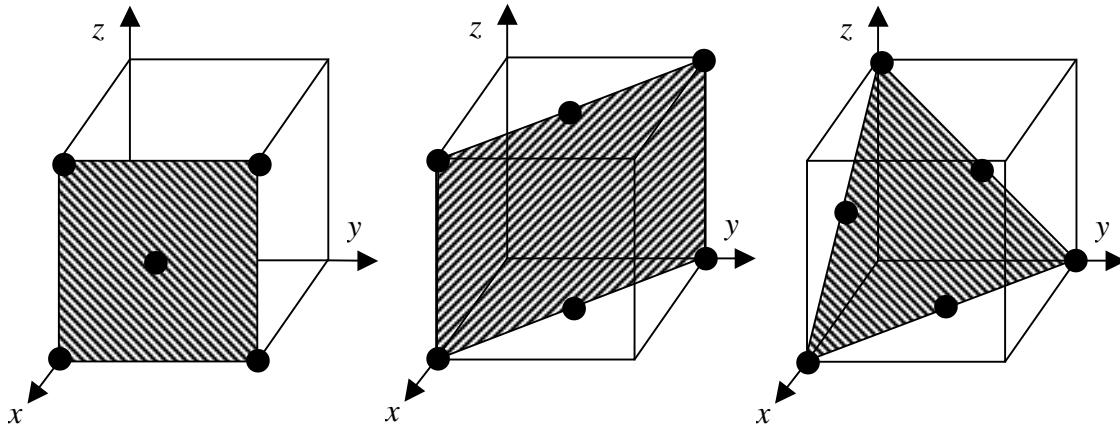
- (a) (100) (b) (110) (c) (111)



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- a. $(1, 0, 0), (1, 0, 1),$
 $(1, 1, 0), (1, 1, 1)$
 $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
- b. $(1, 0, 0), (1, 0, 1),$
 $(0, 1, 0), (0, 1, 1)$
 $(\frac{1}{2}, \frac{1}{2}, 0), (\frac{1}{2}, \frac{1}{2}, 1)$
- c. $(1, 0, 0), (0, 0, 1),$
 $(0, 1, 0), (\frac{1}{2}, 0, \frac{1}{2})$
 $(\frac{1}{2}, \frac{1}{2}, 0), (0, \frac{1}{2}, \frac{1}{2})$

- 3.49 A cubic plane has the following axial intercepts: $a = \frac{1}{3}$, $b = -\frac{2}{3}$, $c = \frac{1}{2}$. What are the Miller indices of this plane?

Given the axial intercepts of $(\frac{1}{3}, -\frac{2}{3}, \frac{1}{2})$, the reciprocal intercepts are:

$\frac{1}{x} = 3$, $\frac{1}{y} = -\frac{3}{2}$, $\frac{1}{z} = 2$. Multiplying by 2 to clear the fraction, the Miller indices are $(6\bar{3}4)$.

- 3.50 A cubic plane has the following axial intercepts: $a = -\frac{1}{2}$, $b = -\frac{1}{2}$, $c = \frac{2}{3}$. What are the Miller indices of this plane?

Given the axial intercepts of $(-\frac{1}{2}, -\frac{1}{2}, \frac{2}{3})$, the reciprocal intercepts are:

$\frac{1}{x} = -2$, $\frac{1}{y} = -2$, $\frac{1}{z} = \frac{3}{2}$. Multiplying by 2, the Miller indices are $(\bar{4}\bar{4}3)$.

- 3.51 A cubic plane has the following axial intercepts: $a = 1$, $b = \frac{2}{3}$, $c = -\frac{1}{2}$. What are the Miller indices of this plane?

Given the axial intercepts of $(1, \frac{2}{3}, -\frac{1}{2})$, the reciprocal intercepts are:

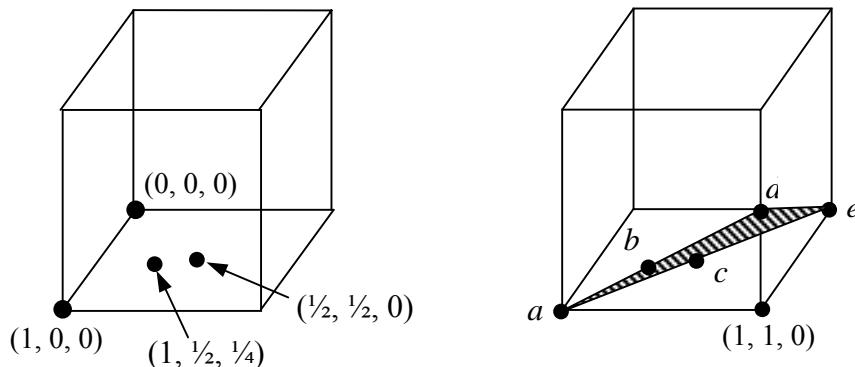
$\frac{1}{x} = 1$, $\frac{1}{y} = \frac{3}{2}$, $\frac{1}{z} = -2$. Multiplying by 2, the Miller indices are $(2\bar{3}\bar{4})$.

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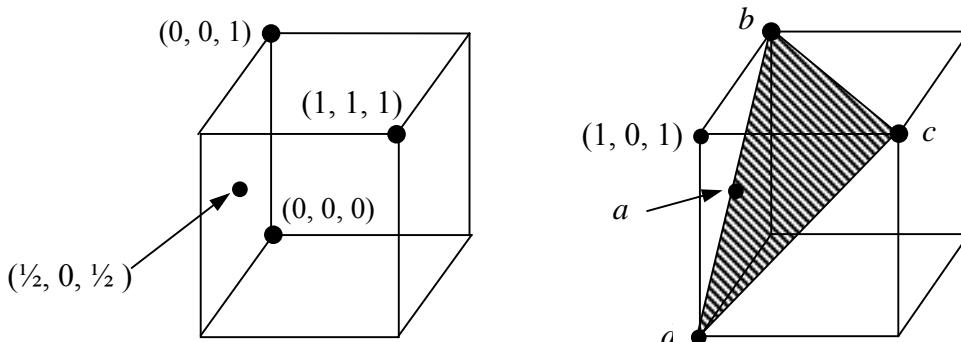
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connecting point d to e . Using $(1, 1, 0)$ as the plane origin, $x = -1$, $y = -1$ and $z = \frac{1}{2}$. The intercept reciprocals are thus $\frac{1}{x} = -1$, $\frac{1}{y} = -1$, $\frac{1}{z} = 2$. The Miller indices are $(\bar{1}\bar{1}2)$.



- 3.53 Determine the Miller indices of the cubic crystal plane that intersects the following position coordinates: $(\frac{1}{2}, 0, \frac{1}{2})$; $(0, 0, 1)$; $(1, 1, 1)$.

First locate the three position coordinates as shown. Next, connect points a and b and extend the line to point d . Complete the plane by connecting point d to c and point c to b . Using $(1, 0, 1)$ as the plane origin, $x = -1$, $y = 1$ and $z = -1$. The intercept reciprocals are thus $\frac{1}{x} = -1$, $\frac{1}{y} = 1$, $\frac{1}{z} = -1$. The Miller indices are $(\bar{1}\bar{1}\bar{1})$.

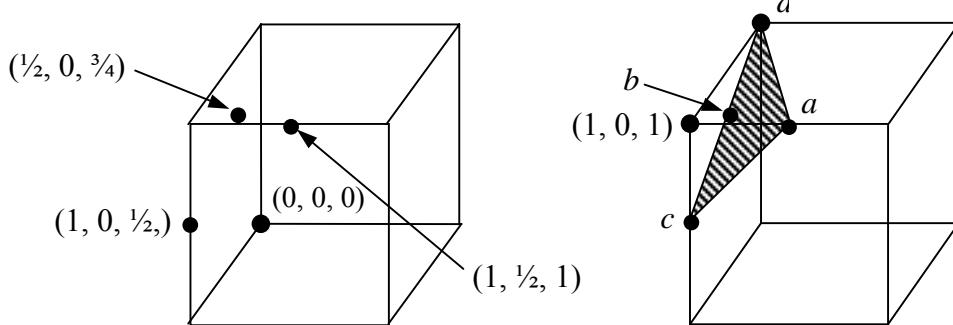


- 3.54 Determine the Miller indices of the cubic crystal plane that intersects the following position coordinates: $(1, \frac{1}{2}, 1)$; $(\frac{1}{2}, 0, \frac{3}{4})$; $(1, 0, \frac{1}{2})$.

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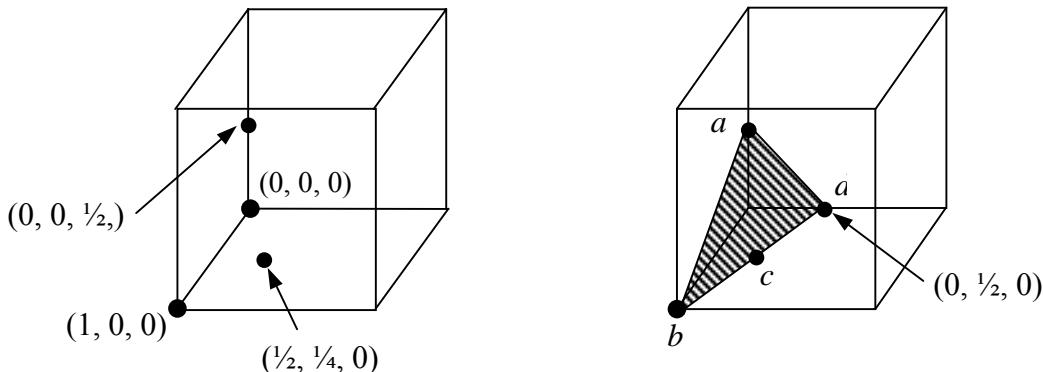
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- 3.55 Determine the Miller indices of the cubic crystal plane that intersects the following position coordinates: $(0, 0, \frac{1}{2})$; $(1, 0, 0)$; $(\frac{1}{2}, \frac{1}{4}, 0)$.

After locating the three position coordinates, connect points b and c and extend the line to point d . Complete the plane by connecting point d to a and a to b . Using $(0, 0, 0)$ as the plane origin, $x = 1$, $y = \frac{1}{2}$ and $z = \frac{1}{2}$. The intercept reciprocals are thus $\frac{1}{x} = 1$, $\frac{1}{y} = 2$, $\frac{1}{z} = 2$. The Miller indices are therefore $(1 \ 2 \ 2)$.



- 3.56 Rodium is FCC and has a lattice constant a of 0.38044 nm. Calculate the following interplanar spacings:
 (a) d_{111} (b) d_{200} (c) d_{220}

$$(a) d_{111} = \frac{0.38044 \text{ nm}}{\sqrt{1^2 + 1^2 + 1^2}} = \frac{0.38044 \text{ nm}}{\sqrt{3}} = 0.220 \text{ nm}$$

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- 3.57 Tungsten is BCC and has a lattice constant a of 0.31648 nm. Calculate the following interplanar spacings:
 (a) d_{110} (b) d_{220} (c) d_{310}

$$(a) d_{110} = \frac{0.31648 \text{ nm}}{\sqrt{1^2 + 1^2 + 0^2}} = \frac{0.31648 \text{ nm}}{\sqrt{2}} = \mathbf{0.224 \text{ nm}}$$

$$(b) d_{220} = \frac{0.31648 \text{ nm}}{\sqrt{2^2 + 2^2 + 0^2}} = \frac{0.31648 \text{ nm}}{\sqrt{8}} = \mathbf{0.112 \text{ nm}}$$

$$(c) d_{310} = \frac{0.31648 \text{ nm}}{\sqrt{3^2 + 1^2 + 0^2}} = \frac{0.31648 \text{ nm}}{\sqrt{10}} = \mathbf{0.100 \text{ nm}}$$

- 3.58 The d_{310} interplanar spacing in a BCC element is 0.1587 nm. (a) What is its lattice constant a ? (b) What is the atomic radius of the element? (c) What could this element be?

$$(a) a = d_{310} \sqrt{h^2 + k^2 + l^2} = (0.1587 \text{ nm}) \sqrt{3^2 + 1^2 + 0^2} = \mathbf{0.502 \text{ nm}}$$

$$(b) R = \frac{\sqrt{3}a}{4} = \frac{\sqrt{3}(0.502 \text{ nm})}{4} = \mathbf{0.217 \text{ nm}}$$

(c) The element is **barium (Ba)**.

- 3.59 The d_{422} interplanar spacing in a FCC metal is 0.083397 nm. (a) What is its lattice constant a ? (b) What is the atomic radius of the metal? (c) What could this metal be?

$$(a) a = d_{422} \sqrt{h^2 + k^2 + l^2} = (0.083397 \text{ nm}) \sqrt{4^2 + 2^2 + 2^2} = \mathbf{0.408 \text{ nm}}$$

$$(b) R = \frac{\sqrt{2}a}{4} = \frac{\sqrt{2}(0.408 \text{ nm})}{4} = \mathbf{0.144 \text{ nm}}$$

(c) The element is **gold (Au)**.

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