Chapter 3, Problem 1

Define the following terms: (a) crystalline solid, (b) long-range order, (c) short-range order, and (d) amorphous.

Chapter 3, Solution 1

(a) a solid that has organized, repeating, 3D positioning of atoms or ions in its structure; (b) the positioning of atoms is periodic and repeating anywhere in the crystal. All atoms have the same geometric environment; (c) there is some order (organized positioning of atoms), but it is local or limited to certain regions of the material; (d) there is no organized positioning of atoms. All atom positions in the structure are random.

Chapter 3, Problem 2

Define the following terms: (a) crystal structure. (b) space lattice, (c) lattice point, (d) unit cell, (e) motif, (f) lattice constants.

Chapter 3, Solution 2

(a) a regular, 3D pattern of atoms or ions in space; (b) a three-dimensional array of points each of which has the same geometric environment; (c) one point in the array in a space lattice; (d) a convenient, smallest, repeating unit of a space lattice; (e) a group of atoms that are organized relative to each other and are associated with a lattice point; (f) length dimensions or angles that characterize geometry of a unit cell.

Chapter 3, Problem 3

What are the 14 Bravais unit cells?

Chapter 3, Solution 3

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.

Chapter 3, Problem 4

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

Chapter 3, Solution 4

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 metals having these structures include the following.

BCC: $\alpha-$iron, vanadium, tungsten, niobium, and chromium.
FCC: copper, aluminum, lead, nickel, and silver.
HCP: magnesium, $\alpha-$titanium, zinc, beryllium, and cadmium.

Chapter 3, Problem 5

For a BBC unit cell, (a) how many atoms are there inside the unit cell, (b) what is the coordination number for the atoms, (c) what is the relationship between the length of the side *a* of the BCC unit cell and the radius of its atoms, and (d) what is the atomic packing factor?

Chapter 3, Solution 5

(a) A BCC crystal structure has **two** atoms in each unit cell. (b) A BCC crystal structure has a coordination number of **eight**. (c) 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 $\sqrt{3}a = 4R$.

Chapter 3, Problem 6

For an FCC unit cell, (a) how many atoms are there inside the unit cell, (b) What is the coordination number fot the atoms, (c) what is the relationship between the length of the side *a* of the FCC unit cell and the radius of its atoms, and (d) what is the atomic packing factor?

Chapter 3, Solution 6

(a) Each unit cell of the FCC crystal structure contains **four** atoms. (b) The FCC crystal structure has a coordination number of **twelve**. (d) 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

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

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,

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

Chapter 3, Problem 7

For an HCP unit cell (consider the primitive cell), (a) how many atoms are there inside the unit cell, (b) What is the coordination number for the atoms, (c) what is the atomic packing factor, (d) what is the ideal *c/a* ratio for HCP metals, and (e) repeat a through c considering the "larger" cell.

Chapter 3, Solution 7

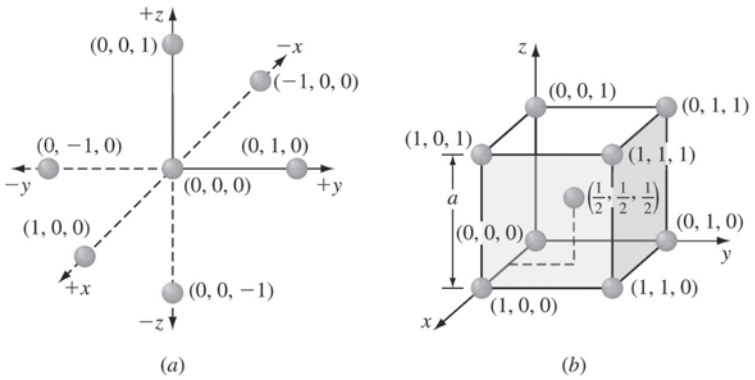
The primitive cell has (a) two atoms/unit cell; (b) The coordination number associated with the HCP crystal structure is **twelve**. (c)the APF is 0.74 or 74%; (d) The ideal *c/a* ratio for HCP metals is **1.633**; (e) all answers remain the same except for (a) where the new answer is 6.

Chapter 3, Problem 8

How are atomic positions located in cubic unit cells?

Chapter 3, Solution 8

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.



Chapter 3, Problem 9

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

Chapter 3, Solution 9

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:
(½, ½, 0), (½, 0, ½), (0, ½, ½), (½, ½, 1), (1, ½, ½), (½, 1, ½)

Chapter 3, Problem 10

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

Chapter 3, Solution 10

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*].

Chapter 3, Problem 11

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

Chapter 3, Solution 11

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

Chapter 3, Problem 12

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

Chapter 3, Solution 12

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.

Chapter 3, Problem 13

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

Chapter 3, Solution 13

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

Chapter 3, Problem 14

How are crystallographic planes indicated in HCP unit cells?

Chapter 3, Solution 14

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 120°; and the vertical c axis.

Chapter 3, Problem 15

What notation is used to describe HCP crystal planes?

Chapter 3, Solution 15

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

Chapter 3, Problem 16

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

Chapter 3, Solution 16

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.

Chapter 3, Problem 17

What are the closest-packed directions in (a) the BCC structure, (b) the FCC structure and (c) the HCP structure?

Chapter 3, Solution 17
(a) The closest packed directions in BCC lattice are $< \bar{1}11 >$ directions.

(b) The closest-packed directions in the FCC lattice are the $< 1\bar{1}0 >$ **directions.**

(c) The closest-packed directions in the HCP lattice are the $< 11\bar{2}0 >$ **directions.**

Chapter 3, Problem 18
Identify the close-packed planes in (a) the BCC structure, (b) the FCC structure, and (c) the HCP structure.

Chapter 3, Solution 18
(a) Does not have a close-packed plane; (b) {111} planes; (c) (0001) planes

Chapter 3, Problem 19
What is polymorphism with respect to metals?

Chapter 3, Solution 19
A metal is considered polymorphic if it can exist in more than one crystalline form under different conditions of temperature and pressure.

Chapter 3, Problem 20
What are X rays, and how are they produced?

Chapter 3, Solution 20
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.

Chapter 3, Problem 21
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.

Chapter 3, Solution 21
See Figure 3.25 of textbook.

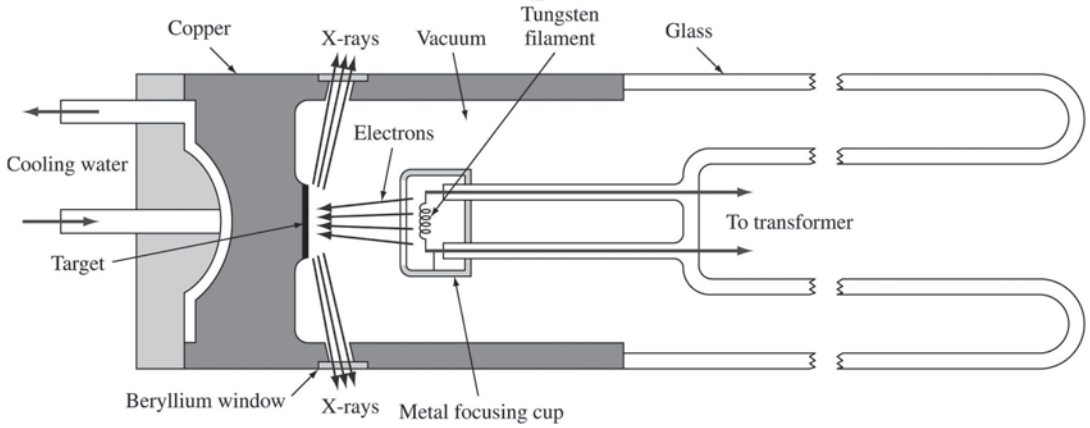


Figure 3.25

Chapter 3, Problem 22
What is the characteristic x-ray radiation? What is its origin?

Chapter 3, Solution 22
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).

Chapter 3, Problem 23
Distinguish between destructive interference and constructive interference of reflected x-ray beams through crystals.

Chapter 3, Solution 23
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.

Application and Analysis Problems

Chapter 3, Problem 24
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.

Chapter 3, Solution 24
Letting a represent the edge length of the BCC unit cell and R the molybdenum atomic radius,

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

Chapter 3, Problem 25
Lithium at 20°C is BCC and has a lattice constant of 0.35092 nm. Calculate a value for the atomic radius of a lithium atom in nanometers.

Chapter 3, Solution 25
For the lithium BCC structure, which has a lattice constant of $a = 0.35092$ nm, the atomic radius is,

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

Chapter 3, Problem 26
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.

Chapter 3, Solution 26
For the gold FCC structure, which has a lattice constant of $a = 0.40788$ nm, the atomic radius is,

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

Chapter 3, Problem 27

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

Chapter 3, Solution 27

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

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

Chapter 3, Problem 28

Verify that the atomic packing factor for the FCC structure is 0.74.

Chapter 3, Solution 28

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

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

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,

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

Chapter 3, Problem 29

Calculate the volume in cubic nanometers of the titanium crystal structure unit cell. Titanium is HCP at 20°C with $a = 0.29504$ nm and $c = 0.46833$ nm.

Chapter 3, Solution 29

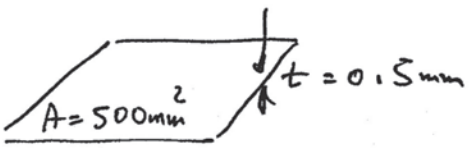
For a hexagonal prism, of height c and side length a, the volume is given by:

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

Chapter 3, Problem 30

Consider a 0.05-mm thick, 500 mm^2 (about three times the area of a dime) piece of aluminum foil. How many units cells exist in the foil? If the density of aluminum is 2.7 g/cm^3, what is the mass of each cell?

3.30



thickness = 0.5 mm Area = $500mm^2$

a) The lattice constant for aluminum is $a = 0.405nm$

$$a = 0.405\ nm = 0.405 \times 10^{-6}\ mm$$

Volume of the sheet = $(A)(t) = (500)(0.5) = 250\ mm^3$

Volume of a single cell = $a^3 = (.405 \times 10^{-6}\ mm)^3$

$$\Rightarrow a^3 = 6.64 \times 10^{-20}\ mm^3$$

$$\#\text{ of unitcell in the sheet} = \frac{250\ mm^3}{6.64 \times 10^{-20}\ mm^3}$$

$$\#\text{ of cells} = 3.76 \times 10^{21}$$

(~ 200 times smaller than the avogardo's #)

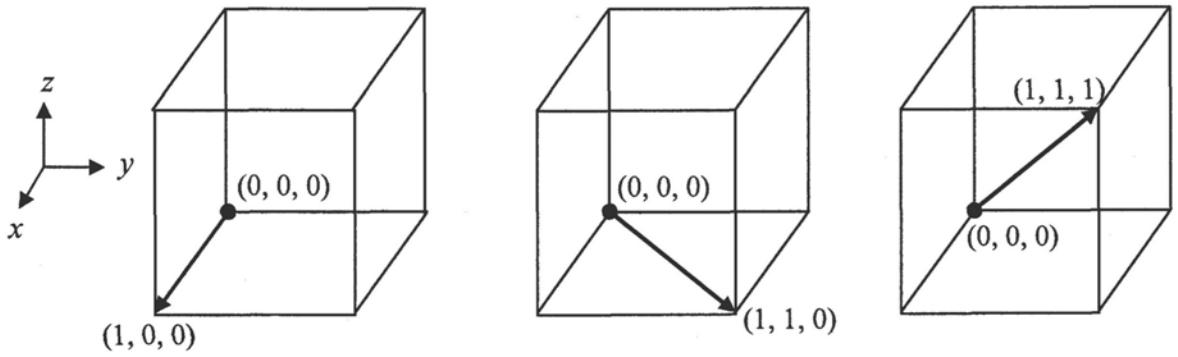
b): $\rho = \frac{m}{V}$

$$m = \rho V = (2.7\ gr/cm^3)\left(6.64 \times 10^{-20}\ mm^3 \times 10^{-3}\ \frac{cm^3}{mm^3}\right)$$

$$m = 1.8 \times 10^{-22}\ gr$$

Chapter 3, Problem 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]

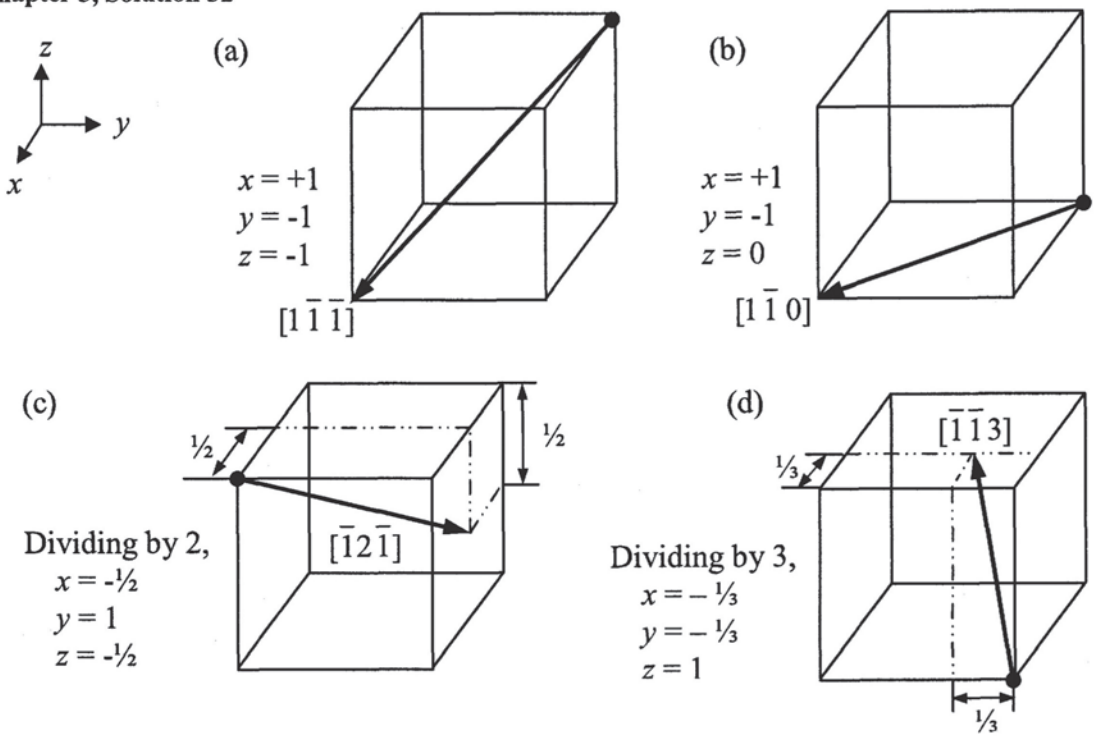
Chapter 3, Solution 31



(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)

Chapter 3, Problem 32
Draw direction vectors in unit cells for the following cubic directions:
(*a*) $[1\bar{1}\bar{1}]$ (*b*) $[1\bar{1}0]$ (*c*) $[\bar{1}2\bar{1}]$ (*d*) $[\bar{1}\bar{1}3]$

Chapter 3, Solution 32



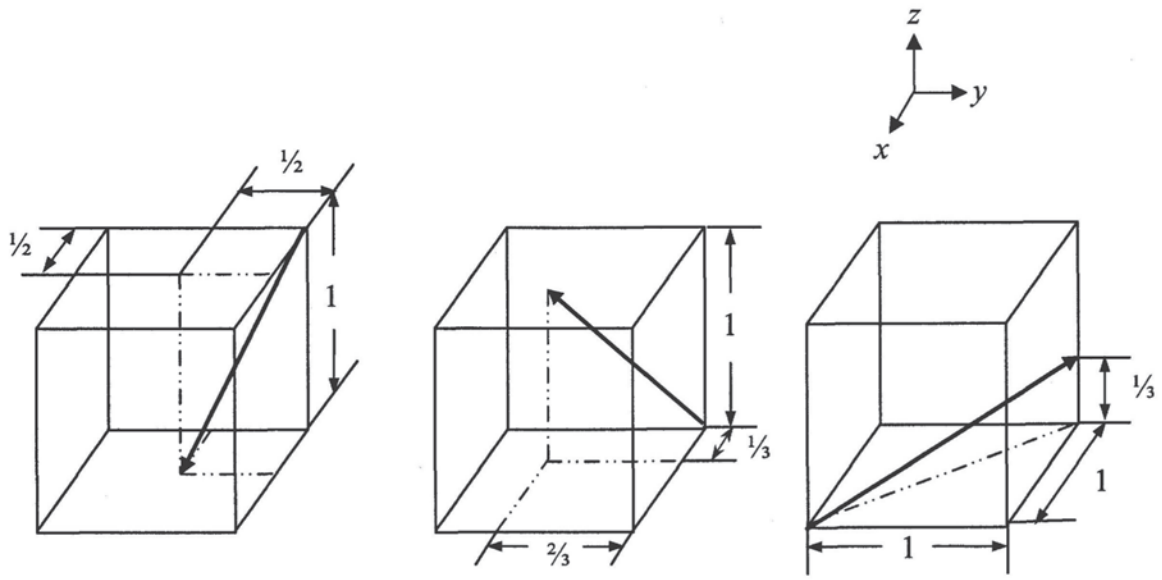
Chapter 3, Problem 33

Draw direction vectors in unit cells for the following cubic directions:

(a) $[1\bar{1}\bar{2}]$ (c) $[\bar{3}31]$ (e) $[2\bar{1}2]$ (g) $[\bar{1}01]$ (i) $[321]$ (k) $[1\bar{2}\bar{2}]$

(b) $[1\bar{2}3]$ (d) $[0\bar{2}1]$ (f) $[2\bar{3}3]$ (h) $[12\bar{1}]$ (j) $[10\bar{3}]$ (l) $[\bar{2}\bar{2}3]$

Chapter 3, Solution 33



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

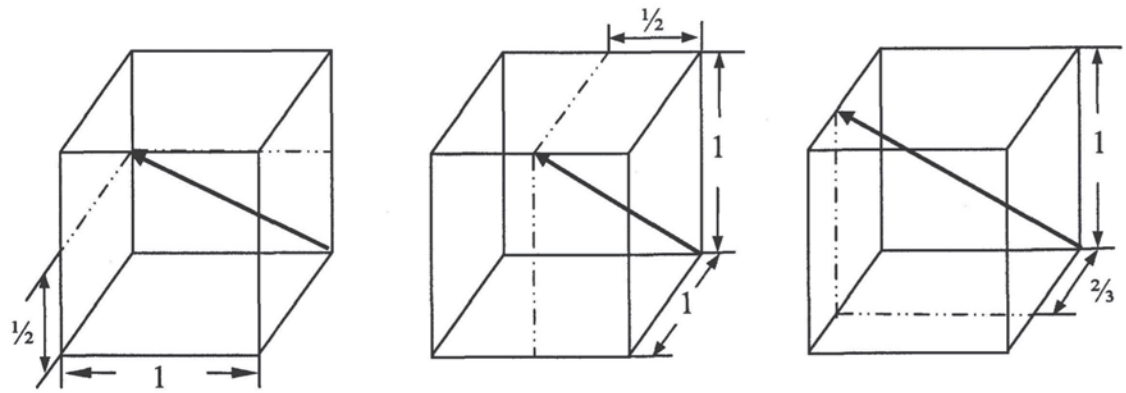
$$x=\frac{1}{2},\ y=-\frac{1}{2},\ z=-1$$

(b) Dividing $[1\bar{2}3]$ by 3,

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

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

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



(d) Dividing $[0\bar{2}1]$ by 2,

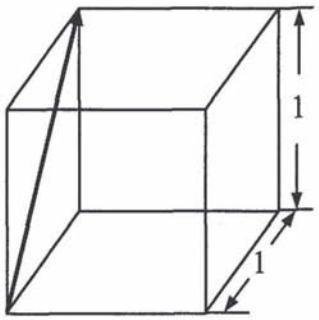
$$x=0,\ y=-1,\ z=\frac{1}{2}$$

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

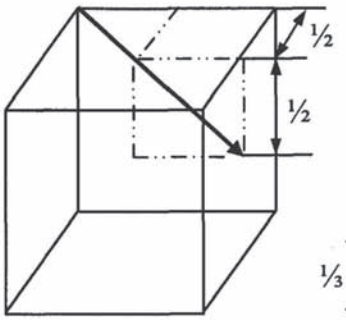
$$x=1,\ y=-\frac{1}{2},\ z=1$$

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

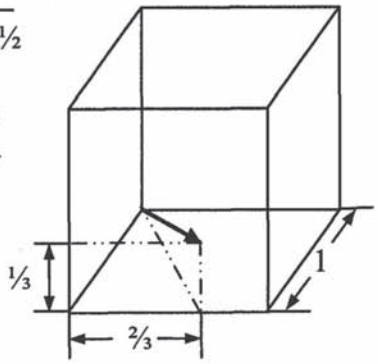
$$x=\frac{2}{3},\ y=-1,\ z=1$$



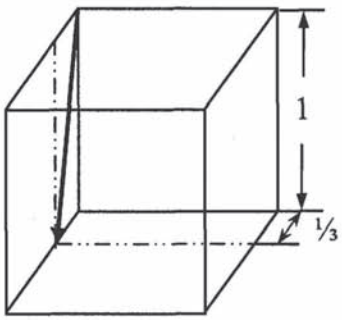
(g) For $[\bar{1}01]$,
$x=-1, y=0, z=1$



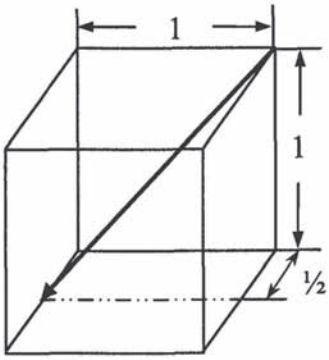
(h) Dividing $[12\bar{1}]$ by 2,
$x=\frac{1}{2}, y=1, z=-\frac{1}{2}$



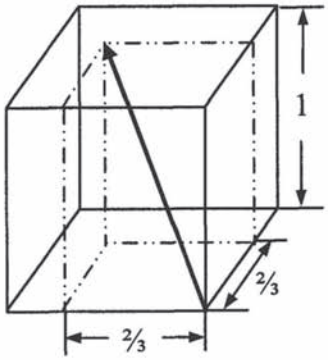
(i) Dividing [321] by 3,
$x=1, y=\frac{2}{3}, z=\frac{1}{3}$



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

Chapter 3, Problem 34
What are the indices of the directions shown in the unit cubes of Fig. P3.34?

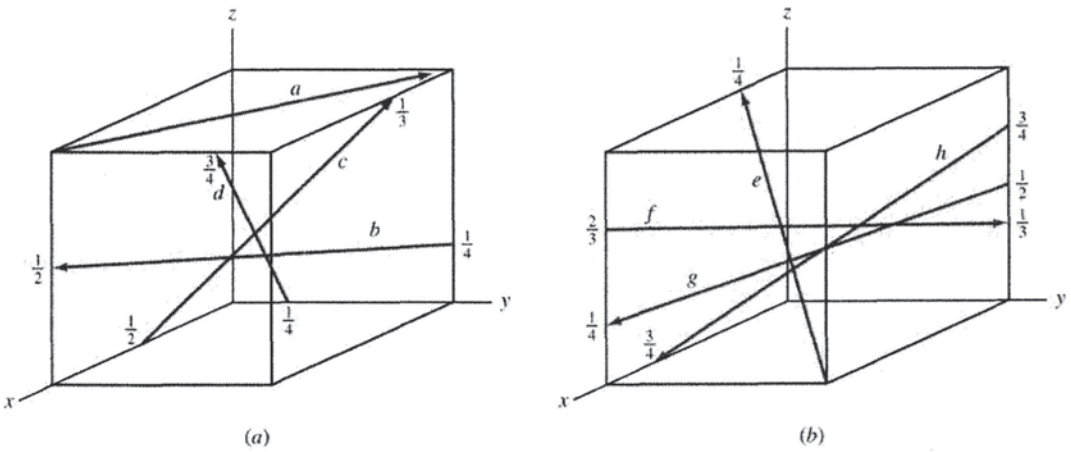
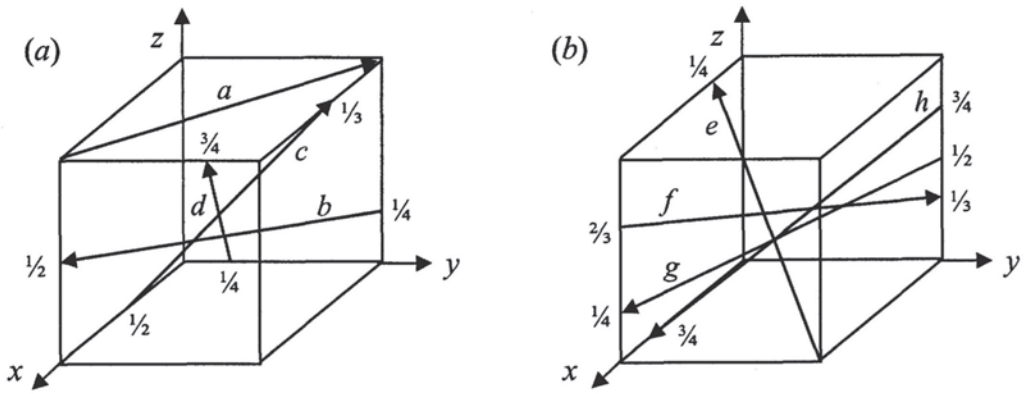
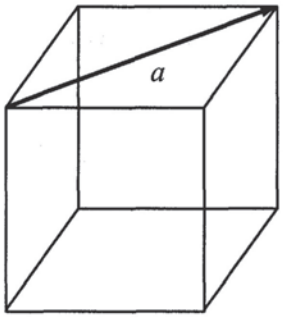
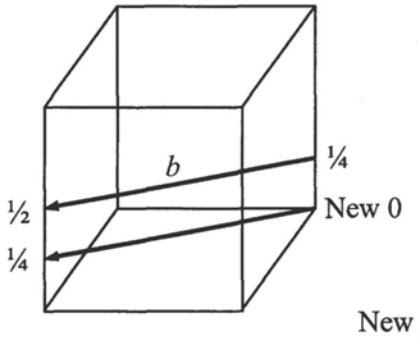


Figure P3.34
Chapter 3, Solution 34

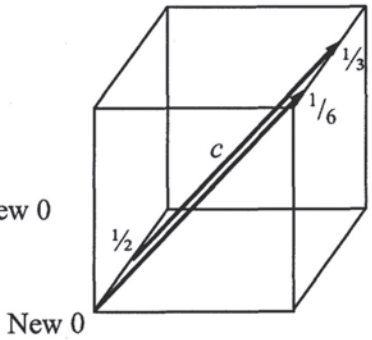




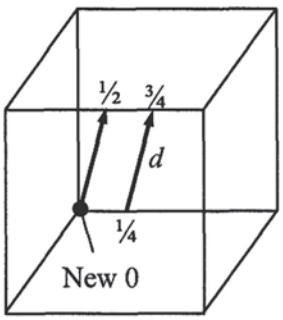
a. Vector components:
$x = -1,\ y = 1,\ z = 0$
Direction indices: $[\bar{1}10]$



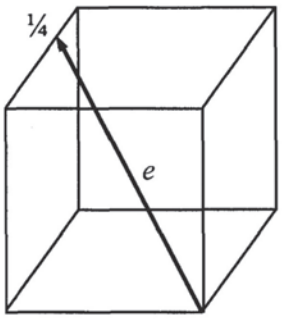
b. Moving direction vector down ¼ , vector components are: $x = 1,\ y = -1,\ z = ¼$
Direction indices: $[4\bar{4}1]$



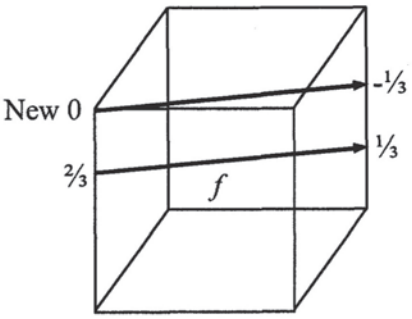
c. Moving direction vector forward ½, vector components are: $x = -⅙,\ y = 1,\ z = 1$
Direction indices: $[\bar{1}66]$



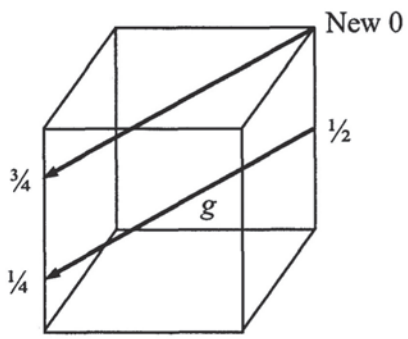
d. Moving direction vector left ¼, vector components are: $x = 1,\ y = ½,\ z = 1$
Direction indices: [212]



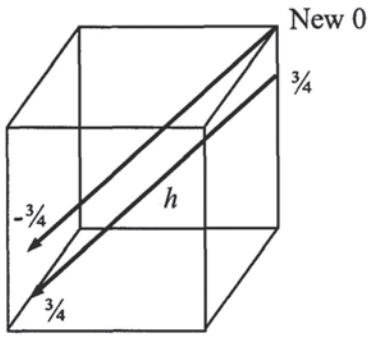
e. Vector components are:
$x = -¾,\ y = -1,\ z = 1$
Direction indices: $[\bar{3}\bar{4}4]$



f. Moving direction vector up ⅓, vector components are:
$x = -1,\ y = 1,\ z = -⅓$
Direction indices: $[\bar{3}3\bar{1}]$



g. Moving direction vector up ½, vector components are: $x = 1,\ y = -1,\ z = -¼$
Direction indices: $[4\bar{4}\bar{1}]$



h. Moving direction vector up ¼, vector components are: $x = ¾,\ y = -1,\ z = -¾$
Direction indices: $[3\bar{4}\bar{3}]$

Chapter 3, Problem 35

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

Chapter 3, Solution 35

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

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

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

Chapter 3, Problem 36

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

Chapter 3, Solution 36

Subtracting coordinates, the vector components are:

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

Clearing fractions through multiplication by 4, gives $x = -3$, $y = 4$, $z = -2$.

The direction indices are therefore $\mathbf{[\bar{3}\,4\,\bar{2}]}$.

Chapter 3, Problem 37

What are the directions of the $[10\bar{3}]$ family or form for a unit cube?

Chapter 3, Solution 37

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

Chapter 3, Problem 38

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

Chapter 3, Solution 38

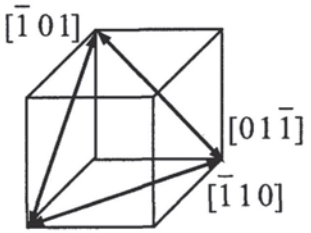
$[111], [\bar{1}\bar{1}\bar{1}], [1\bar{1}1], [\bar{1}1\bar{1}],$
$[\bar{1}11], [1\bar{1}\bar{1}], [11\bar{1}], [\bar{1}\bar{1}1]$

Chapter 3, Problem 39

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

Chapter 3, Solution 39

$[0\bar{1}1], [01\bar{1}], [\bar{1}10], [1\bar{1}0], [\bar{1}01], [10\bar{1}]$

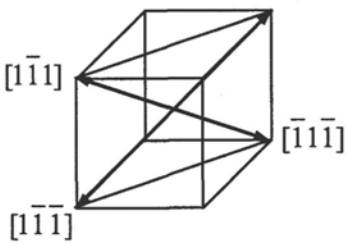


Chapter 3, Problem 40

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

Chapter 3, Solution 40

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



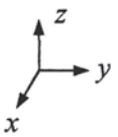
Chapter 3, Problem 41

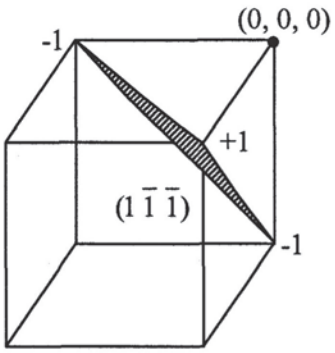
Draw in unit cubes the crystal planes that have the following Miller indices:

(*a*) $(1\bar{1}\bar{1})$ (*c*) $(1\bar{2}\bar{1})$ (*e*) $(3\bar{2}1)$ (*g*) $(20\bar{1})$ (*i*) $(\bar{2}32)$ (*k*) $(3\bar{1}2)$

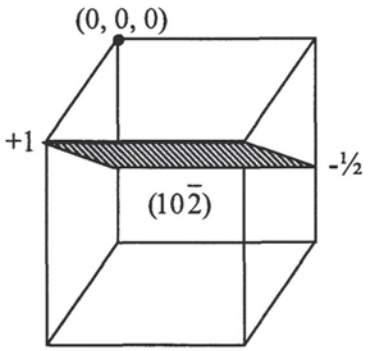
(*b*) $(10\bar{2})$ (*d*) $(21\bar{3})$ (*f*) $(30\bar{2})$ (*h*) $(\bar{2}1\bar{2})$ (*j*) $(13\bar{3})$ (*l*) $(\bar{3}3\bar{1})$

Chapter 3, Solution 41

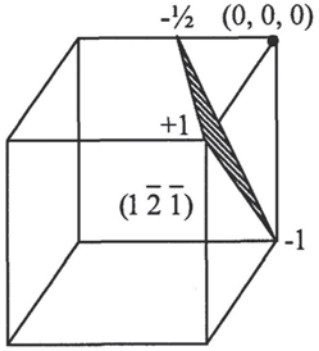




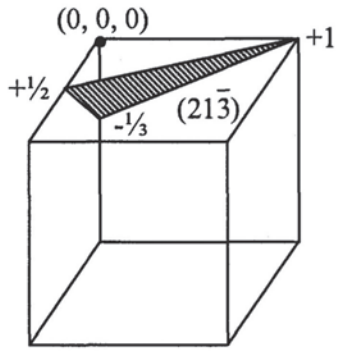
a. For $(1\bar{1}\bar{1})$ reciprocals are: $x = 1,\ y = -1,\ z = -1$



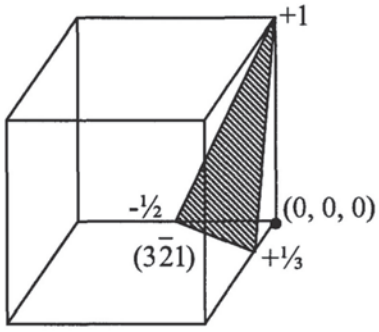
b. For $(10\bar{2})$ reciprocals are: $x = 1,\ y = \infty, z = -½$



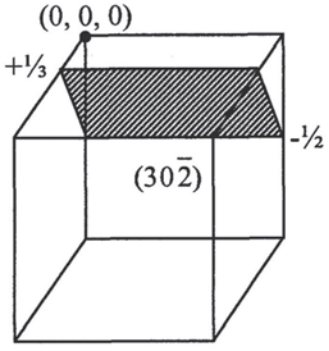
c. For $(1\bar{2}\bar{1})$ reciprocals are: $x = 1,\ y = -½,\ z = -1$



d. For $(21\bar{3})$ reciprocals are: $x = ½,\ y = 1,\ z = -⅓$



e. For $(3\bar{2}1)$ reciprocals are: $x = ⅓,\ y = -½,\ z = 1$



f. For $(30\bar{2})$ reciprocals are: $x = ⅓,\ y = \infty, z = -½$

Chapter 3, Problem 42
What are the Miller indices of the cubic crystallographic planes shown in Fig. P3.42?

Chapter 3, Solution 42

Miller Indices for Figure P3.42(a)

Plane *a* based on (0, 1, 1) as origin

Planar Intercepts	Reciprocals of Intercepts
$x = \infty$	$\frac{1}{x} = 0$
$y = -1$	$\frac{1}{y} = -1$
$z = -\frac{1}{4}$	$\frac{1}{z} = -4$

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

Plane *b* based on (1, 1, 0) as origin

Planar Intercepts	Reciprocals of Intercepts
$x = -1$	$\frac{1}{x} = -1$
$y = \frac{-5}{12}$	$\frac{1}{y} = \frac{-12}{5}$
$z = \infty$	$\frac{1}{z} = 0$

The Miller indices of plane *b* are $(\bar{5}\ \bar{12}\ 0)$.

Plane *c* based on (1, 1, 0) as origin

Planar Intercepts	Reciprocals of Intercepts
$x = \infty$	$\frac{1}{x} = 0$
$y = -1$	$\frac{1}{y} = -1$
$z = \frac{1}{3}$	$\frac{1}{z} = 3$

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

Plane *d* based on (0, 0, 0) as origin

Planar Intercepts	Reciprocals of Intercepts
$x = 1$	$\frac{1}{x} = 1$
$y = 1$	$\frac{1}{y} = 1$
$z = \frac{2}{3}$	$\frac{1}{z} = \frac{3}{2}$

The Miller indices of plane *d* are $(2\ 2\ 3)$.

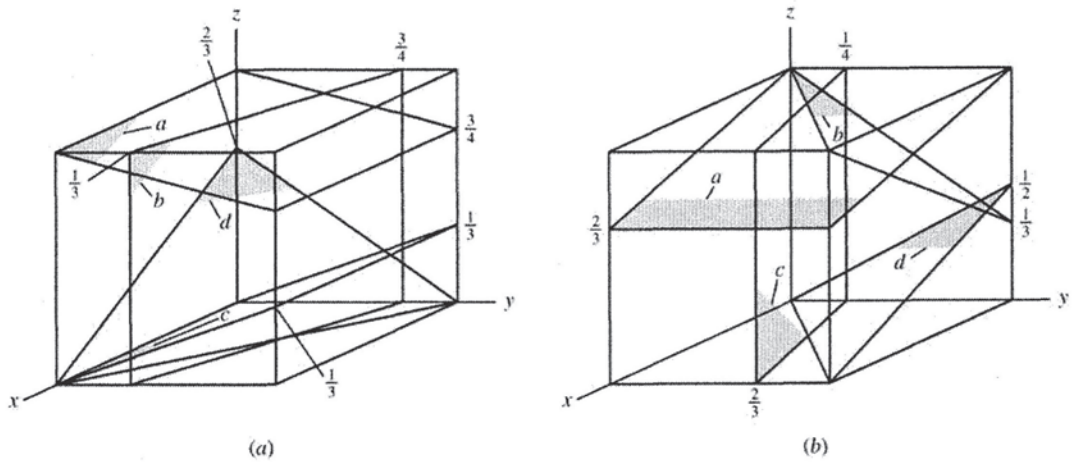


Figure P3.42

Miller Indices for Figure P3.42(b)

Plane *a* based on (1, 0, 1) as origin

Planar Intercepts	Reciprocals of Intercepts
$x = -1$	$\frac{1}{x} = -1$
$y = \infty$	$\frac{1}{y} = 0$
$z = -\frac{1}{3}$	$\frac{1}{z} = -3$

The Miller indices of plane *a* are $(\bar{1}\,0\,\bar{3})$.

Plane *b* based on (0, 1, 1) as origin

Planar Intercepts	Reciprocals of Intercepts
$x = 1$	$\frac{1}{x} = 1$
$y = -1$	$\frac{1}{y} = -1$
$z = -\frac{2}{3}$	$\frac{1}{z} = -\frac{3}{2}$

The Miller indices of plane *b* are $(2\,\bar{2}\,\bar{3})$.

Plane *c* based on (0, 1, 0) as origin

Planar Intercepts	Reciprocals of Intercepts
$x = 1$	$\frac{1}{x} = 1$
$y = \frac{-5}{12}$	$\frac{1}{y} = \frac{-12}{5}$
$z = \infty$	$\frac{1}{z} = 0$

The Miller indices of plane *c* are $(5\,\bar{12}\,0)$.

Plane *d* based on (0, 1, 0) as origin

Planar Intercepts	Reciprocals of Intercepts
$x = 1$	$\frac{1}{x} = 1$
$y = -1$	$\frac{1}{y} = -1$
$z = \frac{1}{2}$	$\frac{1}{z} = 2$

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

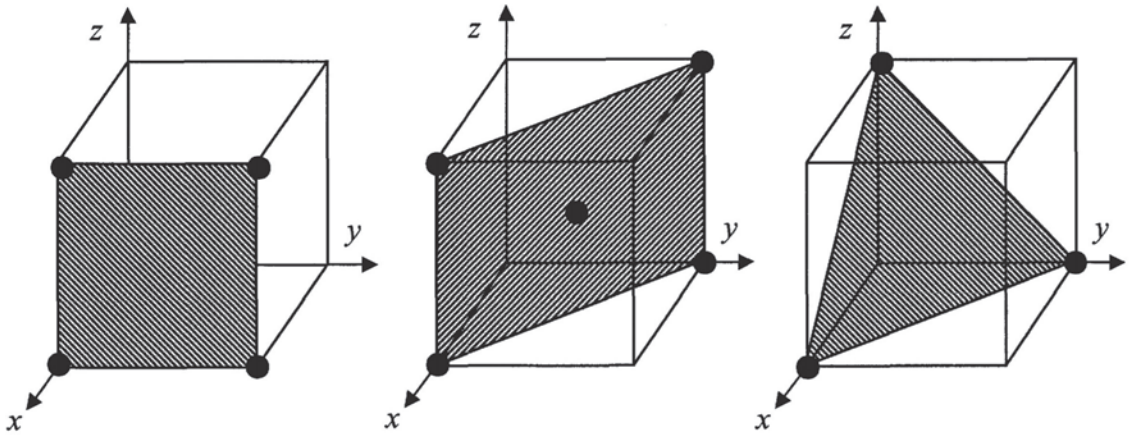
Chapter 3, Problem 43
What are the {100} family of planes of the cubic system?

Chapter 3, Solution 43

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

Chapter 3, Problem 44
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)

Chapter 3, Solution 44



a. (1, 0, 0), (1, 0, 1), (1, 1, 0), (1, 1, 1)

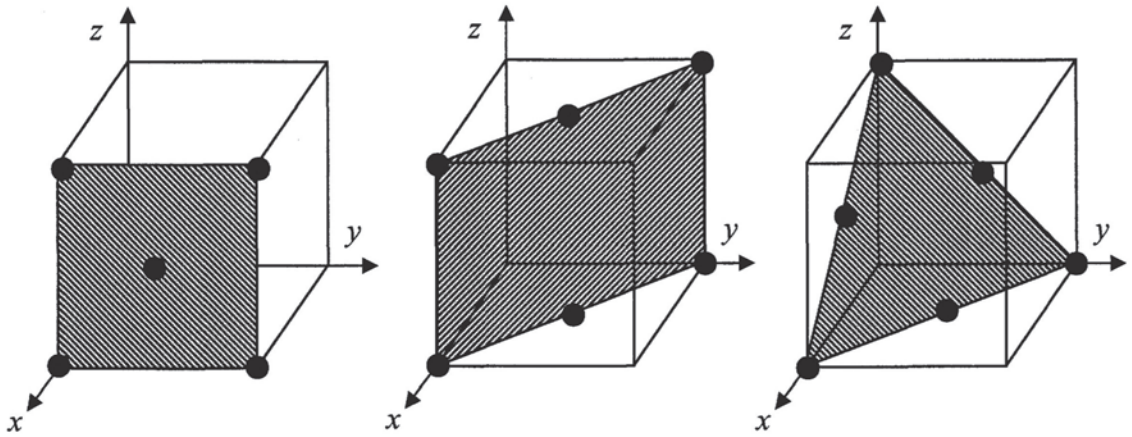
b. (1, 0, 0), (1, 0, 1), (0, 1, 0), (0, 1, 1), (½, ½, ½)

c. (1, 0, 0), (0, 0, 1), (0, 1, 0)

Chapter 3, Problem 45

Draw the following crystallographic planes in an FCC unit cell and list the position coordinates of the atoms whose centers are intersected by each of the planes:
(*a*) (100)(*b*) (110)(*c*) (111)

Chapter 3, Solution 45



a. (1, 0, 0), (1, 0, 1), (1, 1, 0), (1, 1, 1) (1, ½, ½)

b. (1, 0, 0), (1, 0, 1), (0, 1, 0), (0, 1, 1), (½, ½, 0), (½, ½, 1)

c. (1, 0, 0), (0, 0, 1), (0, 1, 0), (½, 0, ½) (½, ½, 0), (0, ½, ½)

Chapter 3, Problem 46

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?

Chapter 3, Solution 46

Given the axial intercepts of (⅓, -⅔, ½), 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 $(6\,\bar{3}\,4)$.

Chapter 3, Problem 47

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?

Chapter 3, Solution 47

Given the axial intercepts of (-½, -½, ⅔), 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 $(\bar{4}\,\bar{4}\,3)$.

Chapter 3, Problem 48

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?

Chapter 3, Solution 48

Given the axial intercepts of (1, ⅔, -½), the reciprocal intercepts are: $\frac{1}{x} = 1,\quad \frac{1}{y} = \frac{3}{2},\quad \frac{1}{z} = -2.$

Multiplying by 2, the Miller indices are $(2\ 3\ \bar{4})$.

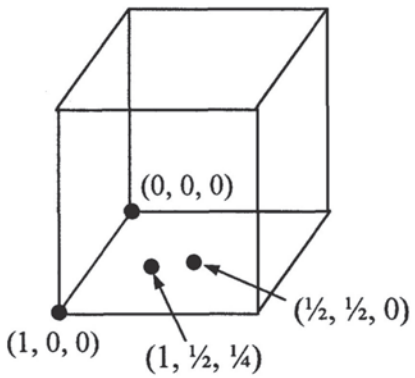
Chapter 3, Problem 49

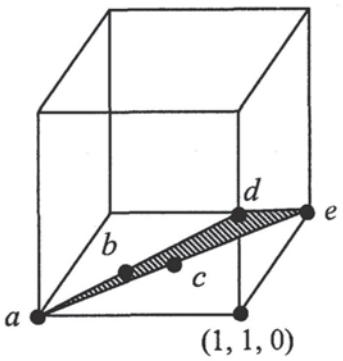
Determine the Miller indices of the cubic crystal plane that intersects the following position coordinates:
$(1, 0, 0);\ (1, \frac{1}{2}, \frac{1}{4});\ (\frac{1}{2}, \frac{1}{2}, 0)$.

Chapter 3, Solution 49

First locate the three position coordinates as shown. Next, connect points *a* and *b,* extending the line to point *d* and connect *a* to *c* and extend to *e*. Complete the plane by connecting point *d* to *e*. Using (1, 1, 0) as the plane origin, $x = -1,\ y = -1$ and $z = ½$. The intercept reciprocals are thus

$\frac{1}{x} = -1,\ \frac{1}{y} = -1,\ \frac{1}{z} = 2.$ The Miller indices are $(\bar{1}\ \bar{1}\ 2)$.





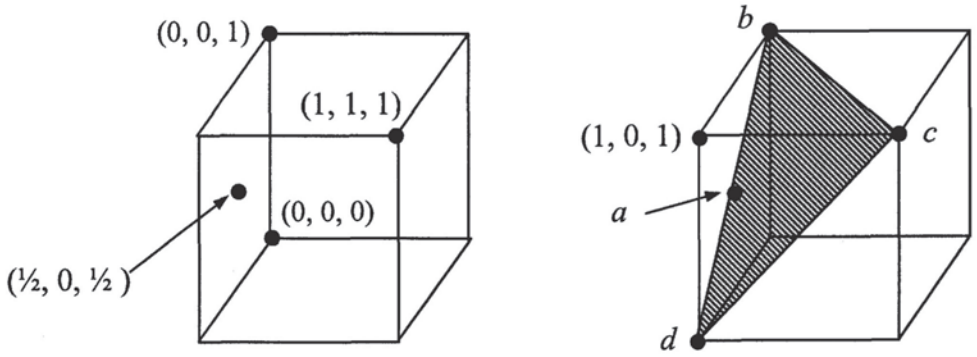
Chapter 3, Problem 50

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

Chapter 3, Solution 50

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 $(\bar{1}\ 1\ \bar{1})$.

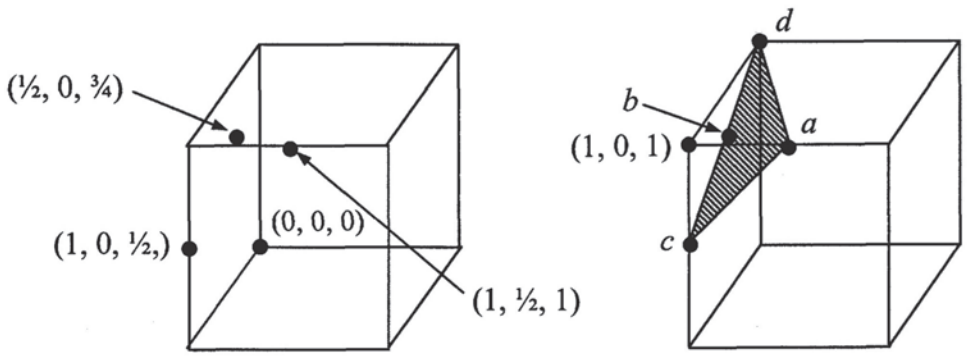


Chapter 3, Problem 51
Determine the Miller indices of the cubic crystal plane that intersects the following position coordinates:
$(1, \frac{1}{2}, 1)$; $(\frac{1}{2}, 0, \frac{3}{4})$; $(1, 0, \frac{1}{2})$.

Chapter 3, Solution 51
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 *c*. Using (1, 0, 1) as the plane origin, $x = -1$, $y = ½$ and $z = -½$. The intercept reciprocals then become

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

The Miller indices are $(\bar{1}\ 2\ \bar{2})$.

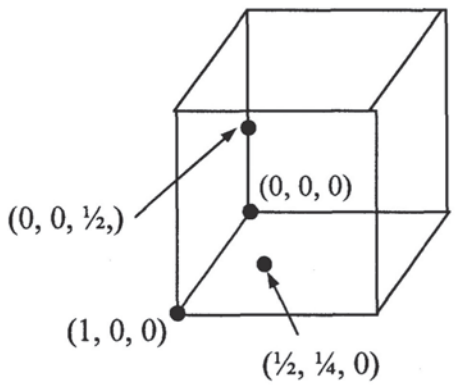


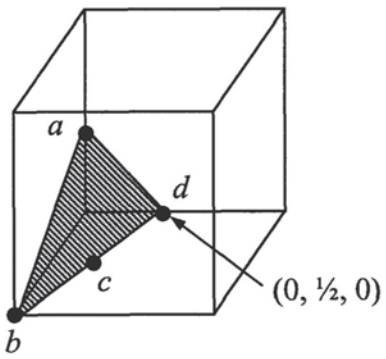
Chapter 3, Problem 52
Determine the Miller indices of the cubic crystal plane that intersects the following position coordinates:
$(0, 0, \frac{1}{2})$; $(1,0,0)$; $(\frac{1}{2},\frac{1}{4},0)$.

Chapter 3, Solution 52
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, $x = 1$, $y = ½$ and $z = ½$. 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)**.





Chapter 3, Problem 53
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}

Chapter 3, Solution 53

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

(b) $$d_{200}=\frac{0.38044\text{ nm}}{\sqrt{2^2+0^2+0^2}}=\frac{0.38044\text{ nm}}{\sqrt{4}}=\mathbf{0.190\text{ nm}}$$

(c) $$d_{220}=\frac{0.38044\text{ nm}}{\sqrt{2^2+2^2+0^2}}=\frac{0.38044\text{ nm}}{\sqrt{8}}=\mathbf{0.135\text{ nm}}$$

Chapter 3, Problem 54
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}

Chapter 3, Solution 54

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

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

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

Chapter 3, Problem 55
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?

Chapter 3, Solution 55

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

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

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

Chapter 3, Problem 56
The d_{422} interplanar spacing in an 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?

Chapter 3, Solution 56

(a) $$a = d_{422}\sqrt{(h^2+k^2+l^2)} = (0.083397)\sqrt{(4^2+2^2+2^2)} = 0.4086\ nm$$

(b) $$R = \frac{a\sqrt{2}}{4} = \frac{0.4086\sqrt{2}}{4} = 0.1445\ nm$$

(c) Closest FCC metal using Appendix II is silver Ag.

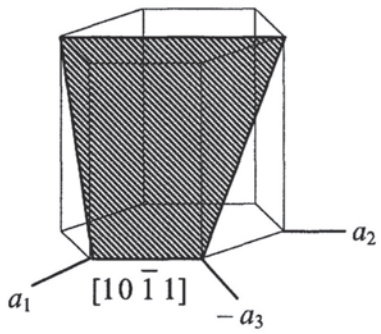
Chapter 3, Problem 57
Draw the hexagonal crystal planes whose Miller-Bravais indices are:

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

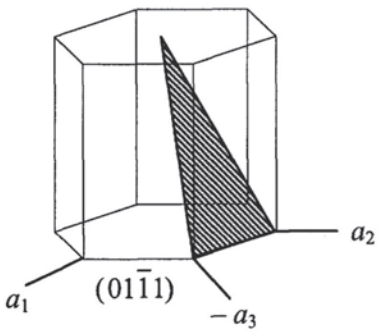
(*b*) $(01\bar{1}1)$ (*e*) $(21\bar{1}1)$ (*h*) $(2\bar{2}00)$ (*k*) $(\bar{2}111)$

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

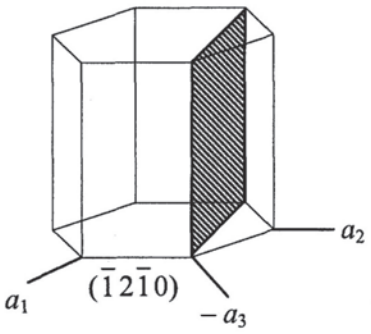
Chapter 3, Solution 57
The reciprocals of the indices provided give the intercepts for the plane (a_1, a_2, a_3, and c).



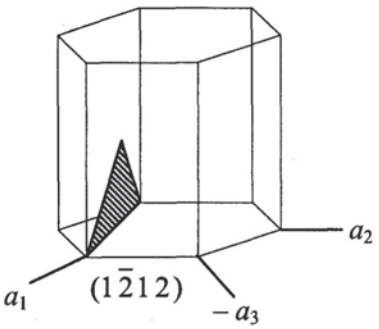
a. $a_1 = 1,\ a_2 = \infty,$
$a_3 = -1,\ c = 1$



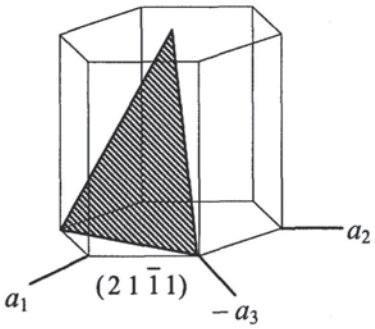
b. $a_1 = \infty,\ a_2 = 1,$
$a_3 = -1,\ c = 1$



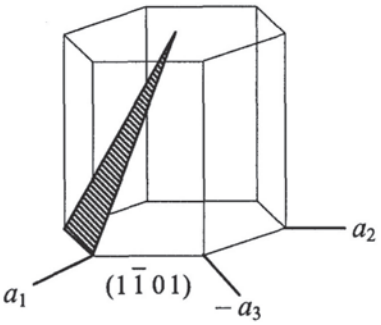
c. $a_1 = 1,\ a_2 = -\frac{1}{2},$
$a_3 = -1,\ c = \infty$



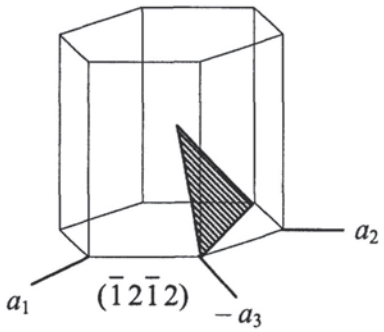
d. $a_1 = 1,\ \ a_2 = -\frac{1}{2},$
$a_3 = 1,\ \ c = \frac{1}{2}$



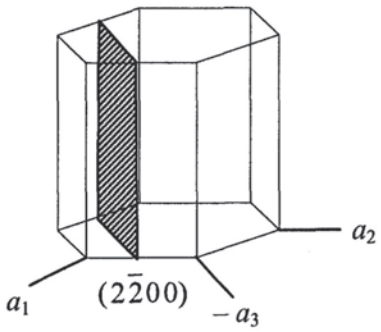
e. $a_1 = \frac{1}{2},\ a_2 = 1,$
$a_3 = -1,\ c = 1$



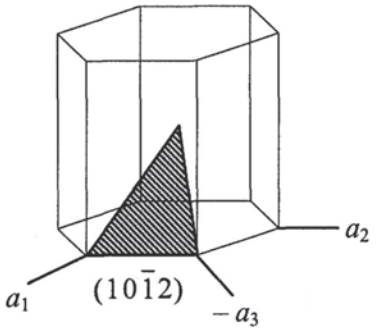
f. $a_1 = 1,\ a_2 = -1,$
$a_3 = \infty,\ c = 1$



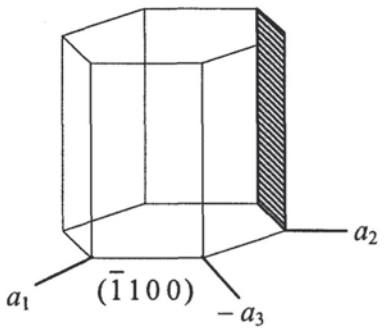
g. $a_1 = -1,\ a_2 = \frac{1}{2},$
$a_3 = -1,\ c = \frac{1}{2}$



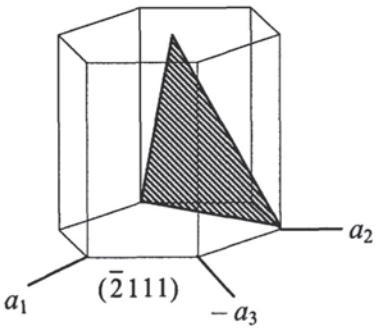
h. $a_1 = \frac{1}{2},\ a_2 = -\frac{1}{2},$
$a_3 = \infty,\ c = \infty$



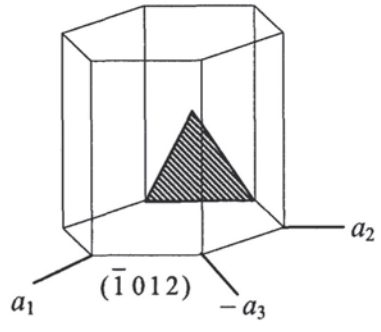
i. $a_1 = 1,\ a_2 = \infty,$
$a_3 = -1,\ c = \frac{1}{2}$



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

Chapter 3, Problem 58
Determine the Miller-Bravais indices of the hexagonal crystal planes in Fig. P3.58.

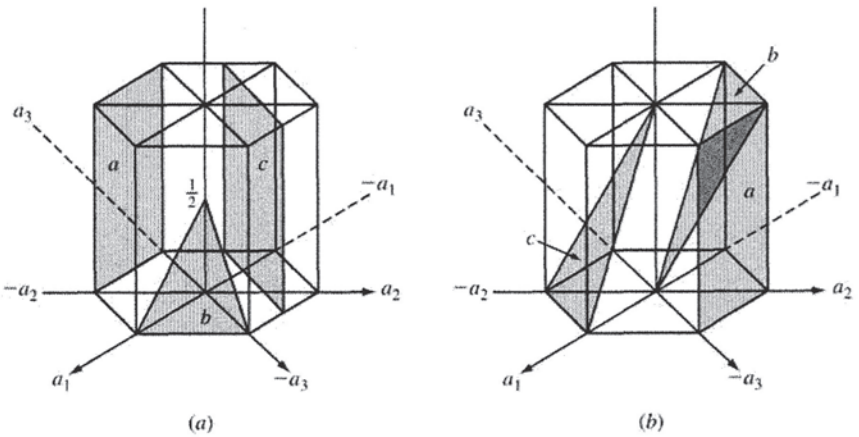


Figure P3.58

Chapter 3, Solution 58

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
$a_1 = \infty$	$\frac{1}{a_1} = 0$	$a_1 = 1$	$\frac{1}{a_1} = 1$	$a_1 = -½$	$\frac{1}{a_1} = -2$
$a_2 = -1$	$\frac{1}{a_2} = -1$	$a_2 = \infty$	$\frac{1}{a_2} = 0$	$a_2 = ½$	$\frac{1}{a_2} = 2$
$a_3 = 1$	$\frac{1}{a_3} = 1$	$a_3 = -1$	$\frac{1}{a_3} = -1$	$a_3 = \infty$	$\frac{1}{a_3} = 0$
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 **$(1\,\bar{1}\,0\,1)$**.	

Chapter 3, Problem 59
Determine the Miller-Bravais direction indices of the $-a_1$, $-a_2$, and $-a_3$ directions.

Chapter 3, Solution 59
The Miller-Bravais direction indices corresponding to the $-a_1$, $-a_2$ and $-a_3$ directions are respectively,
$\left(\frac{1}{4},\ 1,\ \frac{1}{4}\right)$

Chapter 3, Problem 60
Determine the Miller-Bravais direction indices of the vectors originating at the center of the lower basal plane and ending at the endpoints of the upper basal plane as indicated in Fig. 3.16*d*.

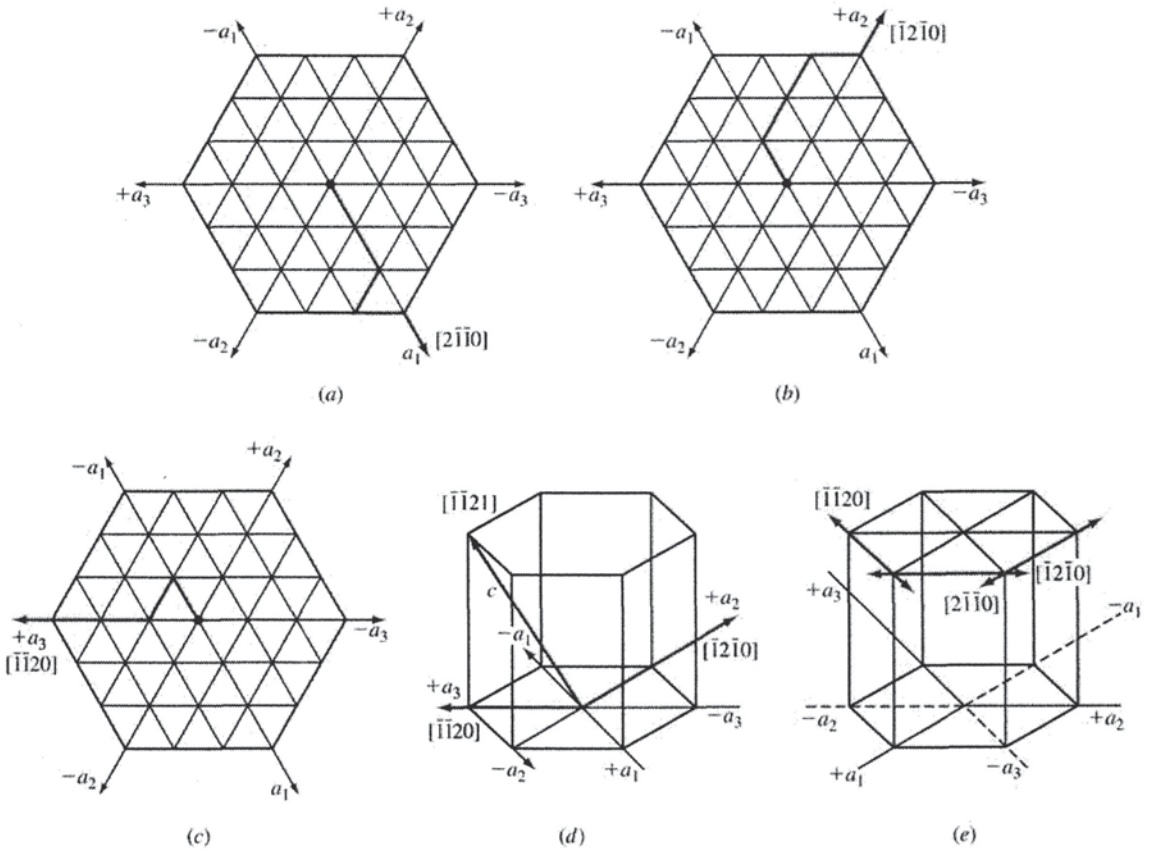
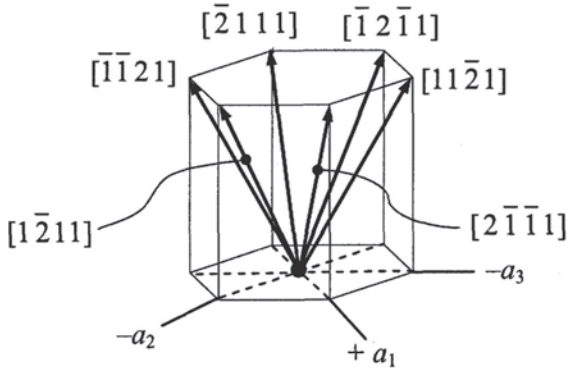


Figure 3.16*d*

Chapter 3, Solution 60

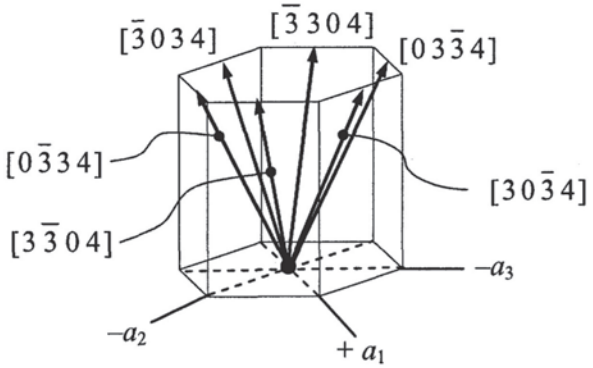
$[\bar{1}\,\bar{1}\,21], [\bar{2}111], [\bar{1}\,2\,\bar{1}\,1],$
$[11\bar{2}1], [2\,\bar{1}\,\bar{1}\,1], [1\,\bar{2}11]$



Chapter 3, Problem 61
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.

Chapter 3, Solution 61

$[\bar{3}\,034], [\bar{3}\,304], [03\bar{3}\,4],$
$[30\bar{3}\,4], [3\bar{3}04], [0\bar{3}34]$



Chapter 3, Problem 62
Determine the Miller-Bravais direction indices of the directions indicated in Fig. P3.62.

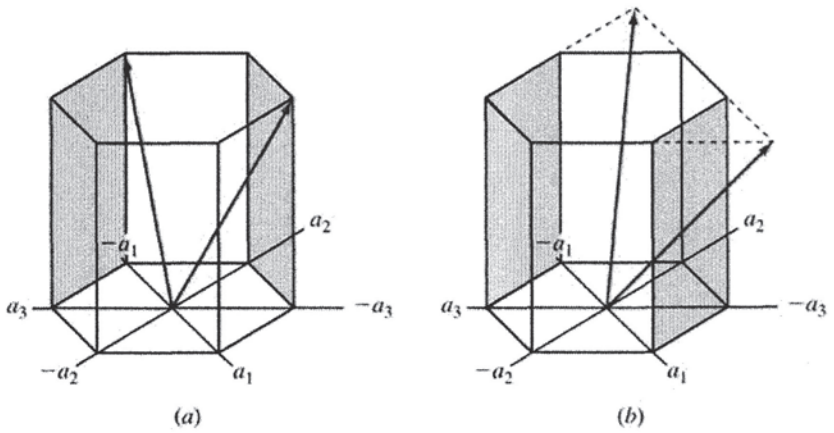
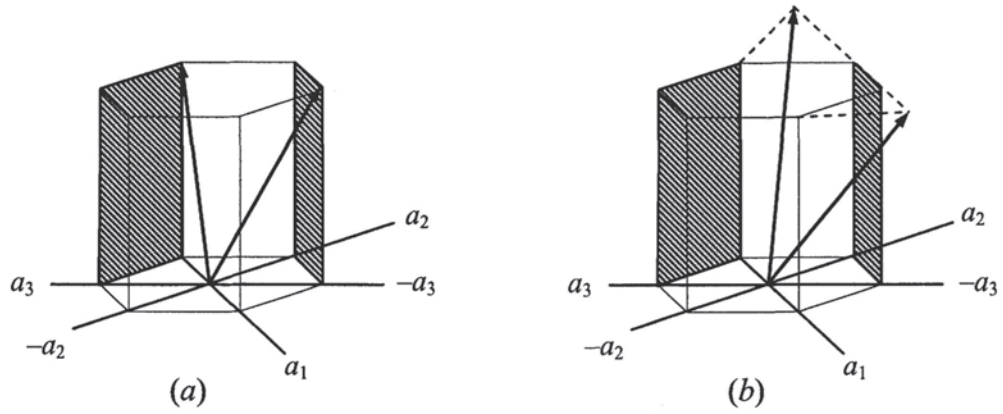


Figure P3.62

Chapter 3, Solution 62



For Fig. P3.62(*a*), the Miller-Bravais direction indices indicated are $[\bar{2}\,1\,1\,1]$ and $[1\,1\,\bar{2}\,1]$. Those associated with Fig. P3.62(*b*) are $[\bar{1}\,1\,0\,1]$ and $[1\,0\,\bar{1}\,1]$.

Chapter 3, Problem 63
The lattice constant for BCC tantalum at 20°C is 0.33026 nm and its density is 16.6 g/cm^3. Calculate a value for its relative atomic mass.

Chapter 3, Solution 63
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:

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

Chapter 3, Problem 64
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.

Chapter 3, Solution 64
First calculate the mass per unit cell based on the atomic mass and the number of atoms per unit cell of the FCC structure,

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

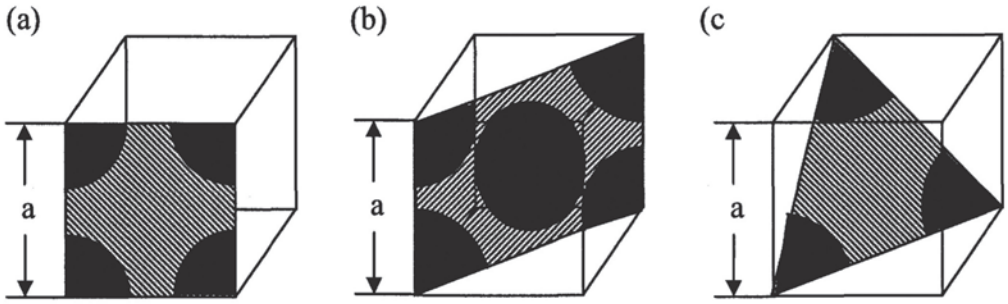
The density is then found as,

$$\rho_v = \frac{\text{mass/unit cell}}{\text{volume/unit cell}} = \frac{\text{mass/unit cell}}{a^3} = \frac{1.296\times10^{-21} \text{ g/unit cell}}{[(0.39239\times10^{-9} \text{ m})^3]/\text{unit cell}}$$

$$= 21,445,113 \text{ g/m}^3 \left(\frac{\text{m}}{100 \text{ cm}}\right)^3 = \mathbf{21.45 \text{ g/cm}^3}$$

Chapter 3, Problem 65
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).

Chapter 3, Solution 65



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,

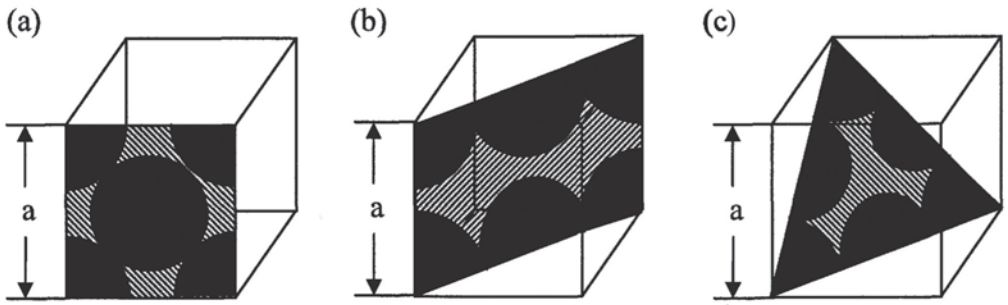
$$\rho_p = \frac{1/2 \text{ atom}}{\frac{\sqrt{6}}{4}(0.28846\times10^{-9} \text{ m})^2} = (9.813\times10^{18} \text{atoms/m}^2)(10^{-6} \text{ m}^2/\text{mm}^2)$$

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

Chapter 3, Problem 66
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).

Chapter 3, Solution 66

(Solutions B and C are on the next page.)



(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,

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

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

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

(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,

$$\rho_p = \frac{2 \text{ atoms}}{\sqrt{2}a^2} = \frac{2}{\sqrt{2}\ (0.40788\times10^{-9}\text{ m})^2} = \mathbf{0.849\times10^{13}\ atoms/mm^2}$$

(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,

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

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

Chapter 3, Problem 67
Calculate the planar atomic density in atoms per square millimeter for the (0001) plane in HCP beryllium, which has a lattice constant a = 0.22856 nm and a c constant of 0.35832 nm.

Chapter 3, Solution 67
The area intersected by the (0 0 0 1) plane and the HCP unit cell is simply the basal area, shown in the sketch to the right:

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

While the number of atoms contained is:

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

The density is therefore,

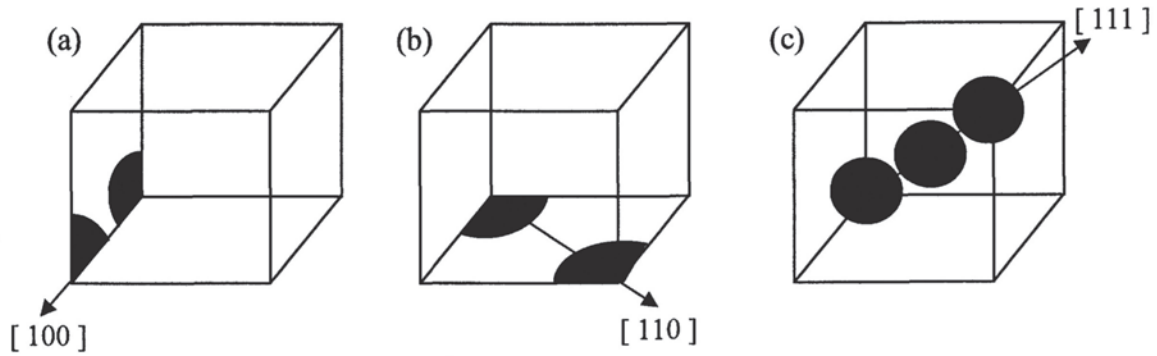
$$\rho_p = \frac{\text{equiv. no. of atoms whose centers are intersected by selected area}}{\text{selected area}}$$

$$= \frac{3 \text{ atoms}}{\frac{3\sqrt{3}}{2}(0.22856\times10^{-9}\text{ m})^2} = (2.201\times10^{19}\text{ atoms/m}^2)\left(\frac{\text{m}}{1000\text{ mm}}\right)^2$$

$$= \mathbf{2.21\times10^{13}\ atoms/mm^2}$$

Chapter 3, Problem 68
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].

Chapter 3, Solution 68



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 BCC vanadium,

$$\rho_l = \frac{\text{no. atom dia.}}{\text{a}} = \frac{1 \text{ atom}}{(0.3039\text{ nm})(10^{-9}\text{ m/nm})(10^3\text{ mm/m})} = \mathbf{3.29\times10^6\ mm}$$

(b) For the [110] direction of BCC vanadium,

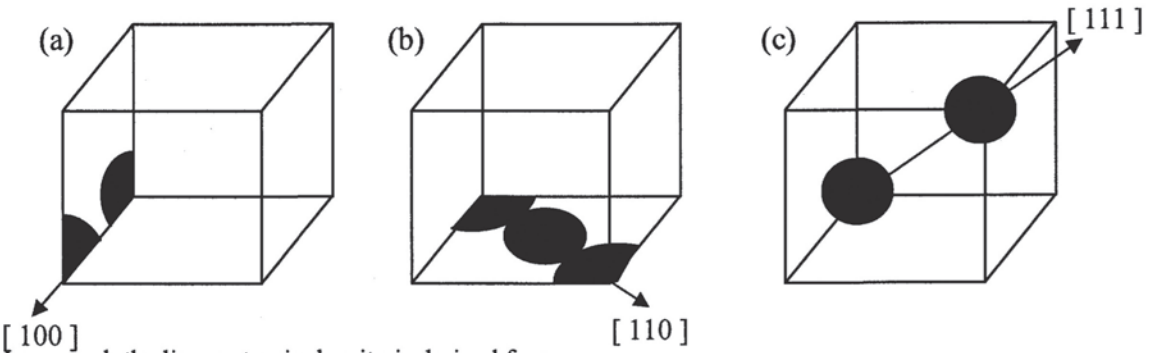
$$\rho_l = \frac{\text{no. atom dia.}}{\sqrt{2}a} = \frac{1 \text{ atom}}{\sqrt{2}(0.3039 \text{ nm})(10^{-6} \text{ mm/nm})} = \mathbf{2.33 \times 10^6 \text{ mm}}$$

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

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

Chapter 3, Problem 69
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].

Chapter 3, Solution 69



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,

$$\rho_l = \frac{\text{no. atom dia.}}{\sqrt{2}a} = \frac{2 \text{ atoms}}{\sqrt{2}(0.38389 \text{ nm})(10^{-6} \text{ mm/nm})} = \mathbf{3.68 \times 10^6 \text{ mm}}$$

(c) For the [111] direction of FCC iridium,

$$\rho_l = \frac{\text{no. atom dia.}}{\sqrt{3}a} = \frac{1 \text{ atom}}{\sqrt{3}(0.38389 \text{ nm})(10^{-6} \text{ mm/nm})} = \mathbf{1.50 \times 10^6 \text{ mm}}$$

Chapter 3, Problem 70
Titanium goes through a polymorphic change from BCC to HCP crystal structure upon cooling through 332°C. 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 882°C is 0.332 nm, and the HCP unit cell has $a = 0.2950$ nm and $c = 0.4683$ nm.

Chapter 3, Solution 70
To determine the volume change, the individual volumes per atom for the BCC and HCP structures must be calculated:

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

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

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

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

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

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

Chapter 3, Problem 71
Pure iron goes through a polymorphic change from BCC to FCC upon heating through 912°C. Calculate the volume change associated with the change in crystal structure from BCC to FCC if at 912°C the BCC unit cell has a lattice constant $a = 0.293$ nm and the FCC unit cell $a = 0.363$ nm.

Chapter 3, Solution 71
First determine the individual volumes per atom for the iron BCC and FCC crystal structures:

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

$$V_{FCC} = \frac{a^3 \text{ nm}^3/\text{unit cell}}{4 \text{ atoms/unit cell}} = \frac{(0.363 \text{ nm})^3}{4 \text{ atoms}} = 0.01196 \text{ nm}^3/\text{atom}$$

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

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

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

Chapter 3, Problem 72

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

Chapter 3, Solution 72

Referring to Fig. 3.25 (*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 interplanar spacing required for constructive interference.

$$MP = d_{hkl} \sin\theta \text{ and } PN = d_{hkl} \sin\theta$$

Substituting,

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

Chapter 3, Problem 73

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 = 88.838°. Calculate a value for the lattice constant *a* for this BCC elemental metal. (Assume first-order diffraction, *n* = 1.)

Chapter 3, Solution 73

The interplanar distance is,

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

The lattice constant, *a*, is then,

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

Chapter 3, Problem 74

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

Chapter 3, Solution 74

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,

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

Chapter 3, Problem 75

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

Chapter 3, Solution 75

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

2θ	θ	$\sin\theta$	$\sin^2\theta$
41.069°	20.535°	0.35077	0.12304
47.782°	23.891°	0.40499	0.16402

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

(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.

Chapter 3, Problem 76

An x-ray diffractometer recorder chart for an element that has either the BCC or the FCC crystal structure showed diffraction peaks at the following 2θ angles:
38.60°, 55.71°, 69.70°, 82.55°, 95.00°, and 107.67°. (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.

Chapter 3, Solution 76

(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

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

(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}.

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

(c) From Appendix I, the BCC metal whose lattice constant is closest to 0.3296 nm is **niobium (Nb)** which has a lattice constant of 0.33007 nm.

Chapter 3, Problem 77

An x-ray diffractometer recorder chart for an element that has either the BCC or the FCC crystal structure showed diffraction peaks at the following 2θ angles:
36.191°, 51.974°, 64.982°, and 76.663°. (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.

Chapter 3, Solution 77

(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

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

(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}.

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

(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.

Chapter 3, Problem 78

An x-ray diffractometer recorder chart for an element that has either the BCC or the FCC crystal structure showed diffraction peaks at the following 2θ angles:
40.663°, 47.314°, 69.144°, and 83.448°. (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.

Chapter 3, Solution 78

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

2θ	θ	$\sin\theta$	$\sin^2\theta$
40.663°	20.3315°	0.34745	0.12072
47.314°	23.657°	0.40126	0.16101

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

(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.

3.79 Do you expect iron and silver to have the same (*a*) atomic packing factor, (*b*) volume of unit cell, (*c*) number of atoms per unit cell, and (*d*) coordination number?

3.79

The answer to all four questions is No since at room temp iron has a BCC unit cell and silver an FCC unit cell. They will have different atomic packing factor, volume of cell, # of atoms per unit cell, and coordination #.

However, above 912°C, iron transforms to FCC structure. Under this condition, we would expect the two metals to have the same atomic packing factor of 0.74, # of atoms per unit cell of 4, and coordination # of 12. But, the cell volume will be different due to differences in atomic radius

3.80 Do you expect gold and silver to have the same (*a*) atomic packing factor, (*b*) volume of unit cell, (*c*) number of atoms per unit cell, and (*d*) coordination number? Verify your answers.

3.80

We expect gold and silver, both FCC, to have the same atomic packing factor (0.74), # of atoms per unit cell (4), and coordination # (12)

The volume of the cell will be larger for the atom with the larger atomic radius. (refer to Table 3.3 for verification)

3.81 Do you expect titanium and silver to have the same (*a*) atomic packing factor, (*b*) volume of unit cell, (*c*) number of atoms per unit cell, and (*d*) coordination number? Verify your answers.

Solution 3.81
Titanium is HCP and Silver is FCC. (a) Both should have the same atomic packing factor of 0.74 although they have different structures. (b) Although they have the same APF, we expect the volume of the cells to be different because the cell geometry and atomic size is different. (c) The number of atoms per unit cell will be different 4 for FCC and 2 for primitive HCP. (d) Coordination # will be the same as in both structures each atom will have 12 neighbors.

***3.82** Show using geometry that the ideal c/a ratio of the hexagonal close-packed unit cell (when atoms are perfect spheres) is 1.633. Hint: draw the center atom in the top basal plane in contact with the three atoms in the center of the HCP cell; connect the centers of the three atoms inside the HCP cell to each other and to the atom at the center of one of the basal planes.

3.82

Connecting the centers of the three atoms in the middle of the HCP cell to each other (atoms 1, 2, and 3) forms the triangle ABC.

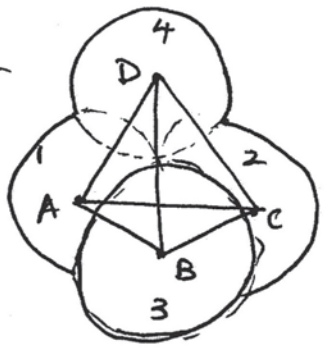


Figure 1

If we now connect the corners A, B, and C to the center of the middle atom in the top basal plane (atom 4), a pyramid ABCD will be formed (Figure 2)

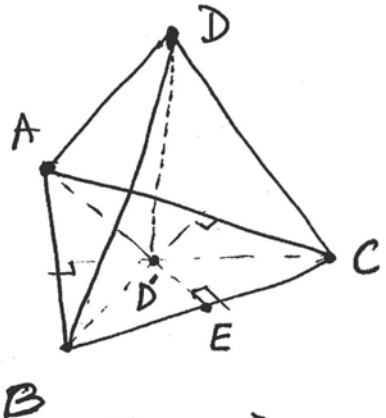


Figure 2.

In this pyramid,

$AB = BC = CA = CD = BD = AD = 2R$

since all atoms are in contact.

If we project point D directly on plane ABC, we will located point D′ (Figure 2). Point D′ is also the intersection of the three heights of ΔABC (Figure 3)

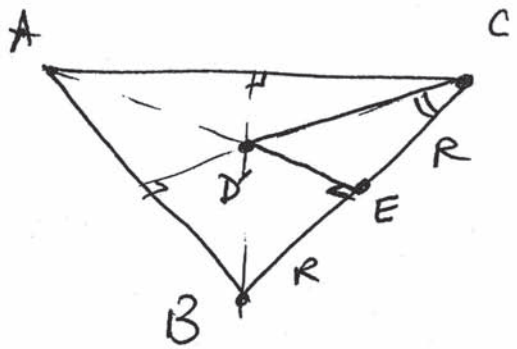


Figure 3

In triangle CED′ (Figure 3)

$CE = R$, then $\frac{R}{CD'} = \cos 30^\circ$

or $CD' = \frac{R}{\cos 30^\circ} = \frac{2R}{\sqrt{3}}$

Now, consider the right triangle $\Delta CD'D'$ in Figure 2.

$$DD'^2 + CD'^2 = CD^2$$

$$\Rightarrow DD'^2 = CD^2 - CD'^2 \quad ; \text{ note } CD = 2R$$

$$DD'^2 = (2R)^2 - \left(\frac{2}{\sqrt{3}}R\right)^2$$

$$DD'^2 = 4R^2 - \frac{4}{3}R^2 = 2\frac{2}{3}R^2 = \frac{8}{3}R^2$$

$$DD' = \sqrt{\frac{8}{3}}\,R = 1.633R$$

note that $\frac{c}{a} = \frac{2DD'}{2R} = \frac{1.633\cancel{R}}{\cancel{R}} = 1.633$

3.83 Assuming that the volume of a HCP metal cell (larger cell) is 0.09130 nm3 and the *c*/*a* ratio is 1.856, determine (*a*) the values for *c* and *a*, and (*b*) the radius, R, of the atom. (*c*) If you were told that the metal is titanium, would you be surprised? How do you explain the discrepancy?

3.83 The volume of an HCP unit cell is

$$V = 3a^2 c \sin 60^\circ \quad \text{(volume of larger cell)}$$

In our problem, $c/a = 1.856 \Rightarrow c = 1.856\,a$

$$\Rightarrow V = 3a^2(1.856a)\sin 60 = 0.09130$$

$$a^3 = \frac{.09130}{(3)(1.856)\left(\frac{\sqrt{3}}{2}\right)} = 0.0189 \text{ nm}^3$$

a) $a = 0.2665$ nm

$$\Rightarrow \quad c = 1.856\,a = 0.4947 \text{ nm}$$

b) $\Rightarrow \quad a = 2R \quad$ or $\quad R = \frac{a}{2} = 0.1333 \text{ nm}$

c) $R_{Zn} = 0.137 \text{ nm}$ from Table 2.11

which greater than our calculated value of 0.133 nm. The zinc atoms are slightly compressed.

***3.84** Assuming that the volume of a HCP metal cell (larger cell) is 0.01060 nm^3 and the *c*/*a* ratio is 1.587, determine (*a*) the values for *c* and *a*, and (*b*) the radius, R, of the atom. (*c*) If you were told that the metal is titanium, would you be surprised? How do you explain the discrepancy?

3.84 The volume of the larger HCP cell is

$$V = 3a^2 c \sin 60^\circ$$

In this problem, $c/a = 1.587 \Rightarrow c = 1.587a$

$$\Rightarrow V = 3a^2(1.587a)\sin 60^\circ = 0.1060\ nm^3$$

$$a^3 = \frac{0.1060}{3(1.587)\left(\frac{\sqrt{3}}{2}\right)} = 0.0257\ nm^3$$

a) $a = 0.2951\ nm$

$$\Rightarrow c = 1.587a = 0.4684\ nm$$

b) $\Rightarrow$ $a = 2R$ or $R = \frac{a}{2} = 0.1476\ nm$

c) $\Rightarrow$ $R_{Ti} = 0.1470$ from Table 2.11

which is slightly smaller than our calculated value of 0.1476 nm. The Ti atoms are slightly elongated.

3.85 The structure of NaCl (an ionic material) is given in Fig. 2.18b. Determine (*a*) its lattice constant *a,* and (*b*) its density. Hint: since NaCl is ionic use the ion radius data and note the atomic radii.

3.85

a) The lattice constant a is

$$a = 2r_{Cl^-} + 2r_{Na^+} = 2(0.095) + 2(0.181)$$

$$a = 0.552\ nm$$

b) The unit cell contains $4\ Na^+$ and $4\ Cl^-$ ions.

Thus, the mass of the cell is

$$m_{cell} = \frac{(4\ Na^+ \times 22.99\ g/mol) + (4Cl^- \times 35.45\ g/mol)}{6.02 \times 10^{23}\ atoms/mol}$$

$$m_{cell} = 3.88 \times 10^{-22}\ gr$$

The volume of the cell is

$$V = a^3 = (0.552\ nm)^3 = 0.1682\ nm^3$$
$$= 1.682 \times 10^{-22}\ cm^3$$

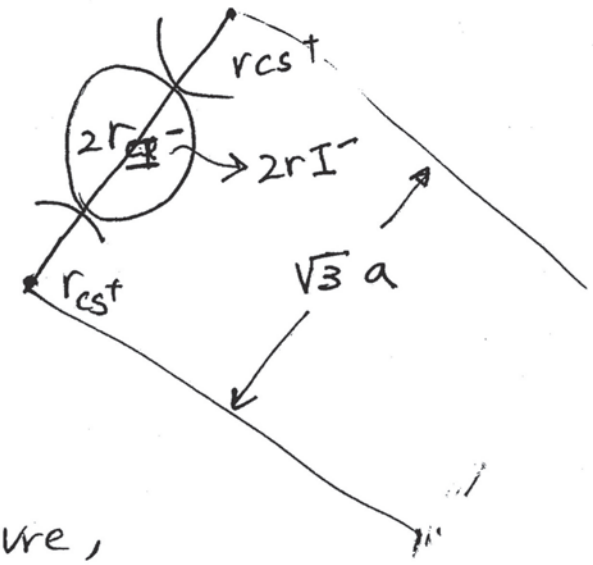
$$\rho = \frac{m}{V} = \frac{3.88 \times 10^{-22}\ g}{1.682 \times 10^{-22}\ cm^3} = 2.31\ \frac{g}{cm^3}$$

The handbook value is $2.16\ g/cm^3$. The difference is mostly due to the underestimated value of Na^+. The radius of Na^+ is ~ 0.102 nm.

3.86 The unit cell structure of the ionic solid, CsI, is similar to that in Fig. 2.18*a*. Determine (*a*) its packing factor, and (*b*) compare this packing factor with that of BCC metals. Explain the difference, if any.

3.86

In figure 2.18 a, Cs^+ and I^- will be in continuous contact along the diagonal of the Cube.



The unit cell contains 1 I^- and 1 Cs^+ ions.

from the figure,

$$\sqrt{3}a = 2r_{Cs^+} + 2r_{I^-}$$

$r_{Cs^+} = 0.169$ nm $\qquad r_{I^-} = 0.216$ nm

Thus,

$$\sqrt{3}a = 2(0.169) + 2(0.216) = 0.770 \text{ nm}$$

$$\boxed{a = 0.445 \text{ nm}}$$

$$APF = \frac{\left[\frac{4}{3}\pi(0.169)^3 + \frac{4}{3}\pi(0.216)^3\right]}{(0.445 \text{ nm})^3} = \frac{.0624 \text{ nm}^3}{.0881 \text{ nm}^3}$$

APF = 0.708 slightly higher than 68% for BCC metals.

3.87 Iron (below 912°C) and tungsten are both BCC with significantly different atomic radii. However, they have the same atomic packing factor of 0.68. How do you explain this?

3.87

Although the radii are significantly different

$R_{Fe} = 0.124\ nm$ $R_W = 0.141\ nm$,

the lattice constants will also be different

$$a_{Fe} = \frac{4R_{Fe}}{\sqrt{2}} \qquad a_W = \frac{4R_W}{\sqrt{2}}$$

a_W will be larger than a_{Fe}.

$$APF = \frac{\text{Volume of atoms inside the cell}}{\text{Volume of the cell}} = \frac{2(\frac{4}{3}\pi R^3)}{a^3}$$

Both numerator and denominator increase for tungsten. Thus keeping the ratio the same.

3.88 Verify that there are eight atoms inside a diamond cubic structure (see Fig. 2.23 *b* and *c*). Draw a 3D schematic of the atoms inside the cell.

3.88

Refering to Figure 2.23 b & c :

- There a eight octants at the eight corners of the cube

- There are six half spheres (hemispheres) at each face

- There are 4 full atoms inside the cell

Thus the total is: $8\left(\frac{1}{8}\right) + 6\left(\frac{1}{2}\right) + 4 = 8 \frac{\text{atoms}}{\text{unit cell}}$

***3.89** The lattice constant for the diamond cubic structure of diamond is 0.357 nm. Diamond is metastable, meaning that it will transform to graphite at elevated temperatures. If this transformation occurs, what % volume change will occur? (Density of graphite is 2.25 gr/cm^3)

3.89

First, let's determine the density of diamond.

From problem 3.88, there are $8 \frac{\text{atoms}}{\text{Unit cell}}$ in a diamond cubic structure. ($a = 0.357$ nm)

Thus $\rho_{diamond} = \dfrac{8\left(\frac{12.01 \text{ gr}}{6.02 \times 10^{23} \text{ atoms/mol}}\right)}{(0.357 \times 10^{-7} \text{ cm})^3} = 3.51 \frac{\text{g.}}{\text{cm}^3}$

$\rho_{graphite} = 2.25 \text{ gr/cm}^3$

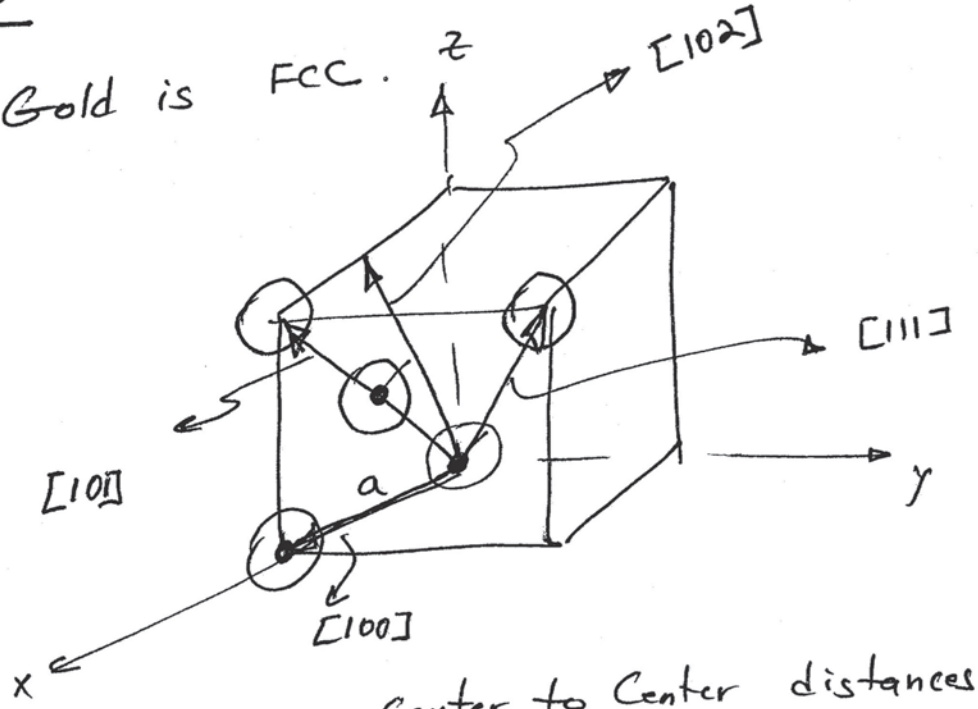
During the transformation, volume will increase

$$\% \text{ increas in volume} = 100 \times \frac{3.51 - 2.25}{3.51} = 35.9\%$$

3.90 Calculate the center-to-center distance between adjacent atoms of gold along the following directions: (*a*) [100], (*b*) [101], (*c*) [111], and (*d*) [102]. Speculate as to why such information may be important in understanding the behavior of the material.

3.90

Gold is FCC.



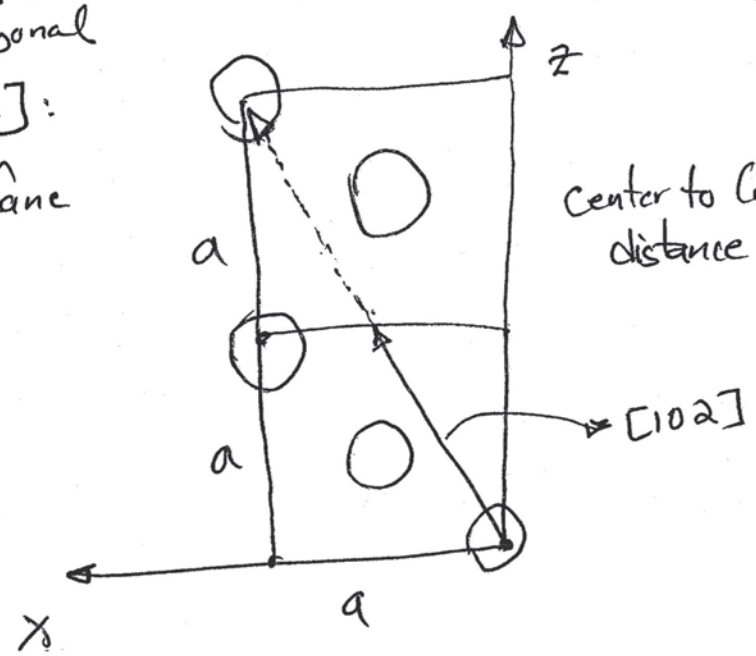
Center to Center distances (one atom at each corner)

[100]: a — cube side

[101]: $\frac{a\sqrt{2}}{2}$ — Face diagonal (one atom at the corner, the next atom at the center of the face)

[111]: $a\sqrt{3}$ — Cube diagonal (one atom at each corner of cube diagonal)

[102]: direction in x-z plane



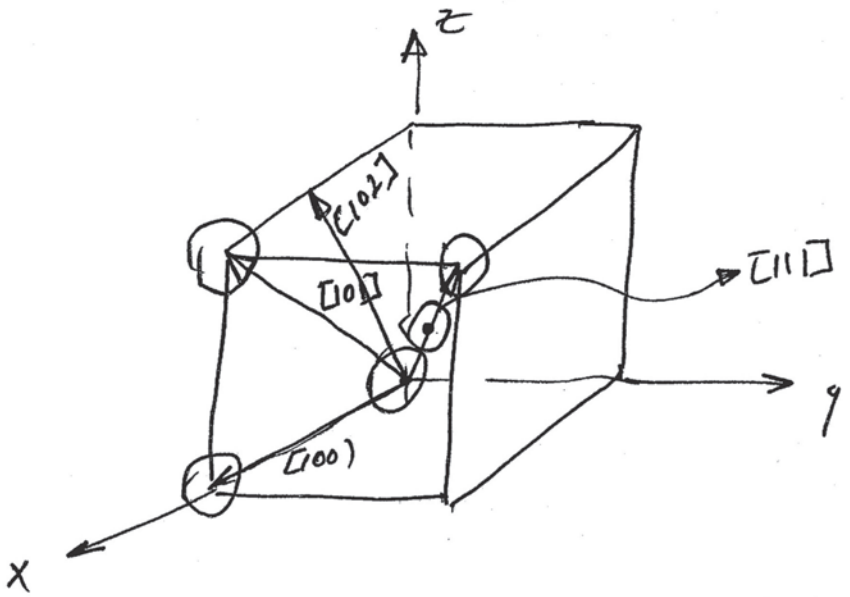
Center to Center distance $= \sqrt{a^2+(2a)^2} = \sqrt{5a^2} = \sqrt{5}\,a$

- when planes of atom slip on top of each other, the [101] direction will be the most efficient slip direction since the atoms are closest to each other.
[102] will be the least efficient direction for slip.

***3.91** Calculate the center-to-center distance between adjacent atoms of tungsten along the following directions: (*a*) [100], (*b*) [101], (*c*) [111], and (*d*) [102]. Speculate as to why such information may be important in understanding the behavior of the material.

3.91

Tungsten is BCC.

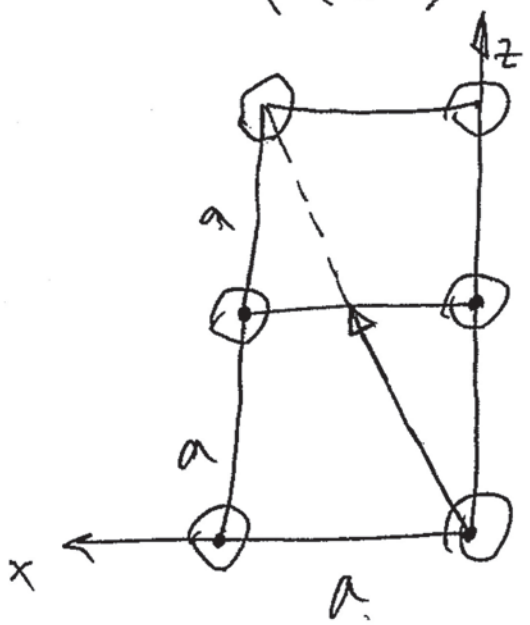


Center to Center distances

[100] : a . (one atom at each corner)
cube side

[101] : $a\sqrt{2}$ (or $1.14a$) (one atom at each corner)
Face diagonal

[111] : $a\frac{\sqrt{3}}{2}$ (or $\left(\frac{1.73}{2}\right)a$) (one atom at the corner, the next atom at the center of the cube)
cube diagonal



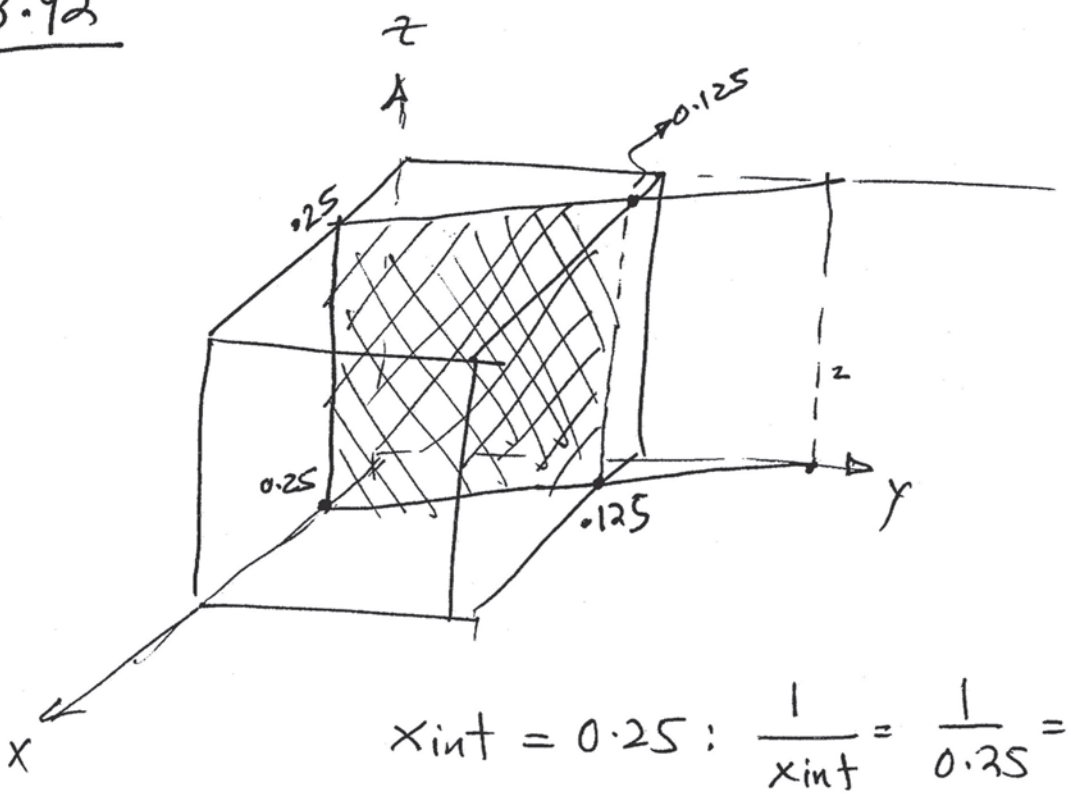
[102]

Center to Center distance $= \sqrt{a^2 + (2a)^2} = \sqrt{5}\,a$ (or $2.23a$)

- The most efficient direction for slip is the [111], due to smallest interatomic distance.

3.92 A plane in a cubic crystal intersects the *x* axis at 0.25, the *y* axis at 2, and is parallel to the *z* axis. What are the miller indices for this plane? Draw this plane in a single cube and show all key dimensions.

3.92



$x_{int} = 0.25: \quad \frac{1}{x_{int}} = \frac{1}{0.25} = 4$

$y_{int} = 2: \quad \frac{1}{y_{int}} = \frac{1}{2} = 0.5$

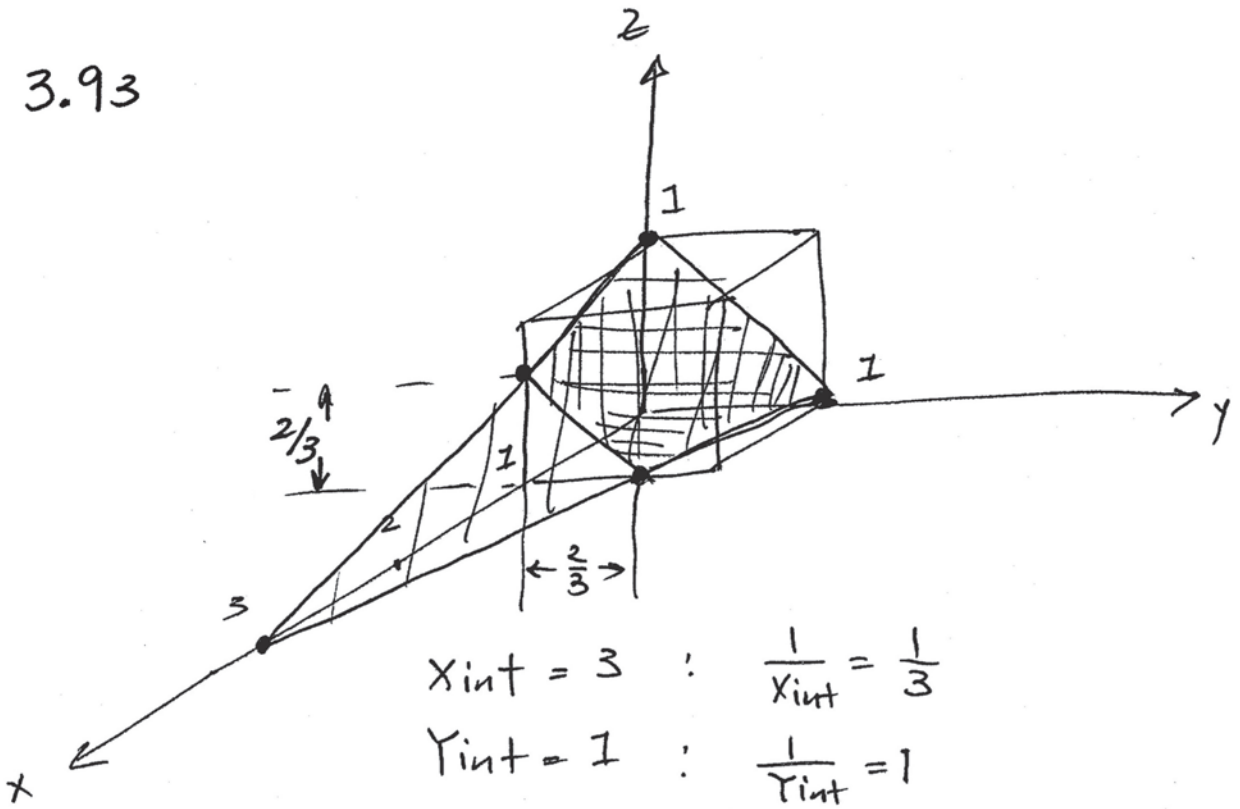
$z_{int} = \infty: \quad \frac{1}{\infty} = 0$

multiply through by 2 to gid rid of fractions.

$\Rightarrow$ The plane is (8 1 0)

3.93 A plane in a cubic crystal intersects the *x* axis at 3, the *y* axis at 1, and the *z* axis at 1. What are the miller indices for this plane? Draw this plane in a single cube and show all key dimensions.

3.93



$X_{int} = 3 : \quad \frac{1}{X_{int}} = \frac{1}{3}$

$Y_{int} = 1 : \quad \frac{1}{Y_{int}} = 1$

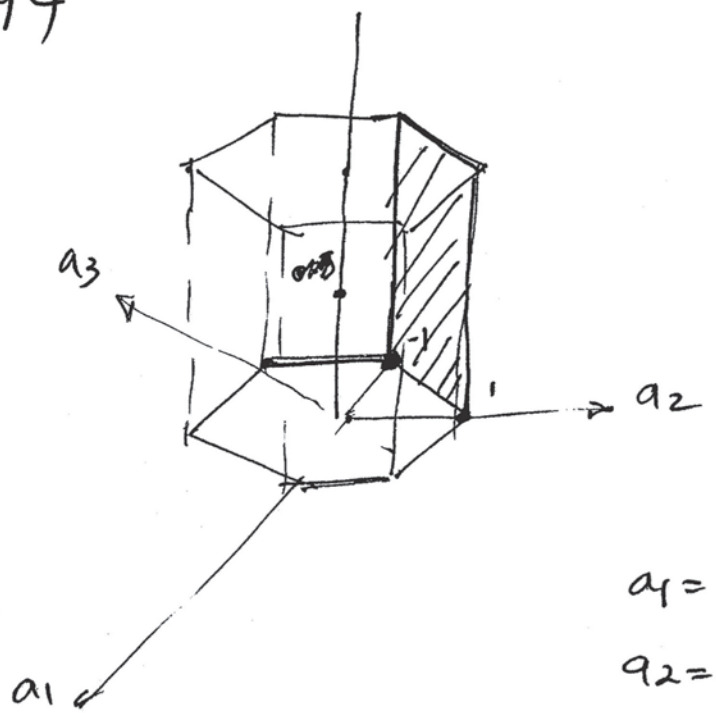
$Z_{int} = 1 : \quad \frac{1}{Z_{int}} = 1$

multiply through by 3 to get rid of fractions

The plane is (1 3 3).

3.94 A plane in a hexagonal crystal intersects at the a_1 axis at -1, the a_2 axis at 1 and the c axis at infinity? What are the Miller indices for this plane? Draw this plane in a hexagonal unit cell and show all key dimensions.

3.94



$a_1 = -1 \Rightarrow h = -1$

$a_2 = 1 \Rightarrow k = 1$

$c = \infty \Rightarrow l = 0$

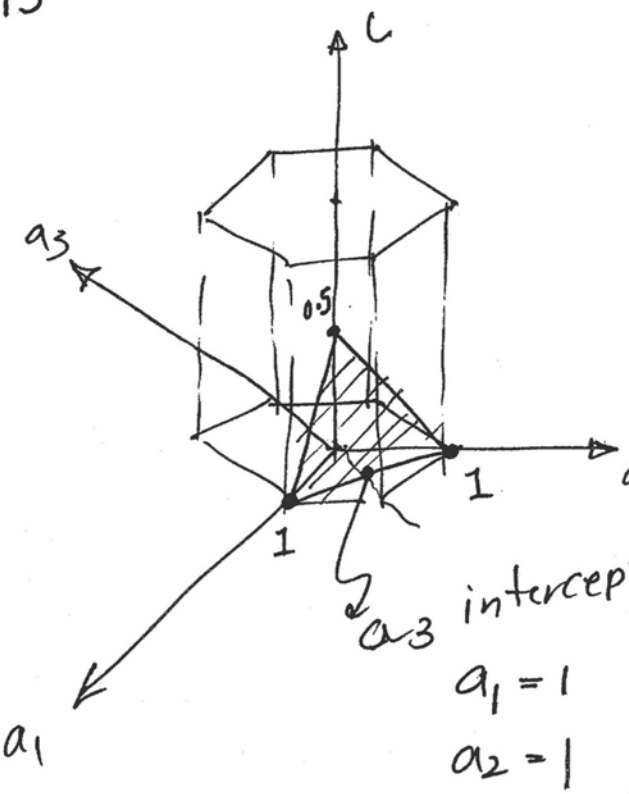
$a_3 = h + k = -i \Rightarrow i = -(h+k)$

$i = -(-1+1) = 0$

$\Rightarrow (\bar{1}100)$

3.95 A plane in a hexagonal crystal intersects at the a_1 axis at 1, the a_2 axis at 1 and the c axis at 0.5? What are the Miller indices for this plane? Draw this plane in a hexagonal unit cell and show all key dimensions.

3.95



a_3 intercept is -0.5

$a_1 = 1 \Rightarrow h = 1$

$a_2 = 1 \Rightarrow k = 1$

$c = 0.5 \Rightarrow l = 2$

$i = -(h+k) = -(1+1) = -2$

a) $a_3 = -\frac{1}{2} \Rightarrow$ The plane is $(1\,1\,\bar{2}\,2)$

b) $a_3 = -0.5$

***3.96** Without drawing any of the hexagonal planes given below, determine which of the planes is, in fact, not a plane. (*a*) $(\bar{1}0\bar{1}0)$, (*b*) $(10\bar{1}0)$, and (*c*) $(\bar{1}\bar{1}0)$.

3.96

a) $h+k=-i$ $\quad (-1+0) \neq -(-1)$

$-1 \neq 1$ (impossible plane)

b) $h+k=-i$ $\quad (1+0) = -(-1)$

$1 = 1$ (plane exists)

c) $h+k=-i$ $\quad (-1+1) \neq -(-1)$

$0 \neq +1$ (impossible plane)

3.97 Name as many carbon allotropes as you can, and discuss their crystal structure.

3.97

- grahite is layered hexagonal
- diamond is diamond cubic
- bucky ball is cage similar to soccer ball with 60 c atoms (there are other forms as well)
- buck tube is a long tube with hexagonal shapes
- coal or soot is amorphous.

3.98 A thin layer of aluminum nitride is sometimes deposited on Silicon wafers at high temperatures (1000°C). The coefficient of thermal expansion and the lattice constant of the silicon crystal is different than that of aluminum nitride. Will this cause a problem? Explain.

3.98

- Yes, this could cause a problem. As the temperature is lowered or as the substrate cools, the two materials (Silicon & Aluminum Nitride) will contract at different levels or magnitudes.
- This could cause cracking of the substrate due to thermal residual stresses.

3.99 An unknown material is being analyzed using X-ray diffraction techniques. However, the diffraction patterns are extremely broad (no clear peaks are visible). (*a*) What does this tell you about the material? (*b*) What are some of the tests that you can perform to help identify the material or narrow the possibilities?

3.99

(a) The material is amorphous or glassy.

(b) measure its density, magnetic properties, electrical properties, strength, spectrometry (to determine the make up)

3.100 Explain, in general terms, why many polymers and some ceramic glasses have an amorphous or semicrystalline structure.

3.100

There are factors that inhibit the formation of a periodic ordered arrangment of atoms or molecules in certain materials thus causing formation of amorphous structures.

In polymers, the major factor is the the secondary bonds between molecules which will not allow for tight and parallel positiong of molecules everywhere in the material.

existence

In ceramic glasses, even a modest cooling rate will stop the progression of crystallization and the glass will become amorphous.

3.101 Explain how ultra-rapid cooling of some metal alloys produces metallic glass.

3.101

Metals, unlike ceramic glasses, crystallize (form a crystal structure) from a molten state very rapidly. In order to stop the rapid crystallization process, one would have to apply extremely fasting cooling rates to freeze the atoms in their disordered state while in molten state.