Chapter 3, Problem 1

Define a crystalline solid.

Chapter 3, Solution 1

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.

Chapter 3, Problem 2

Define a crystal structure. Give examples of materials that have crystal structures.

Chapter 3, Solution 2

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.

Chapter 3, Problem 3

Define a space lattice.

Chapter 3, Solution 3

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

Chapter 3, Problem 4

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

Chapter 3, Solution 4

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.

Chapter 3, Problem 5

What are the 14 Bravais unit cells?

Chapter 3, Solution 5

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 6

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

Chapter 3, Solution 6

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 7

How many atoms per unit cell are there in the BCC crystal structure?

Chapter 3, Solution 7

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

Chapter 3, Problem 8

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

Chapter 3, Solution 8

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

Chapter 3, Problem 9

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

Chapter 3, Solution 9

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 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.

Chapter 3, Solution 10

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

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

Chapter 3, Problem 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.

Chapter 3, Solution 11

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

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

Chapter 3, Problem 12

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 12

For the lithium BCC structure, which has a lattice constant of a = 0.35092 nm, the atomic radius is,

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

Chapter 3, Problem 13

Sodium at 20°C is BCC and has a lattice constant of 0.42906 nm. Calculate a value for the atomic radius of a sodium atom in nanometers.

Chapter 3, Solution 13

For the sodium BCC structure, with a lattice constant of a = 0.42906 nm, the atomic radius is,

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

Chapter 3, Problem 14

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

Chapter 3, Solution 14

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

Chapter 3, Problem 15

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

Chapter 3, Solution 15

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

Chapter 3, Problem 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.

Chapter 3, Solution 16

For the gold FCC structure, which has a lattice constant of a = 0.40788 nm, the atomic radius is,

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

Chapter 3, Problem 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.

Chapter 3, Solution 17

For the platinum FCC structure, with a lattice constant of a = 0.39239 nm, the atomic radius is,

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

Chapter 3, Problem 18

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 18

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

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

Chapter 3, Problem 19

Strontium is FCC and has an atomic radius of 0.215 nm. Calculate a value for its lattice constant *a* in nanometers.

Chapter 3, Solution 19

For an FCC unit cell having an edge length *a* an containing strontium atoms,

$$\sqrt{2}a = 4R \quad \text{or} \quad a = \frac{4}{\sqrt{2}}R = \frac{4}{\sqrt{2}}(0.215 \text{ nm}) = \mathbf{0.608\,nm}$$

Chapter 3, Problem 20

Calculate the atomic packing factor for the FCC structure.

Chapter 3, Solution 20

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 21

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

Chapter 3, Solution 21

The hexagonal prism contains **six** atoms.

Chapter 3, Problem 22

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

Chapter 3, Solution 22

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

Chapter 3, Problem 23

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

Chapter 3, Solution 23

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

Chapter 3, Problem 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?

Chapter 3, Solution 24

Cadmium and zinc have significantly higher *c/a* ratios while zirconium, titanium, magnesium, cobalt and beryllium have slightly lower ratios.

Chapter 3, Problem 25

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 25

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

$$V = (\text{Area of Base})(\text{Height}) = [(6 \times \text{Equilateral Triangle Area})(\text{Height})]$$

$$= (3a^2 \sin 60^o)(c)$$

$$= 3(0.29504\ \text{nm})^2 (\sin 60^o)(0.46833\ \text{nm})$$

$$= \mathbf{0.106\ nm^3}$$

Chapter 3, Problem 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. Calculate a value for its lattice constant *a* in nanometers.

Chapter 3, Solution 26

The rhenium lattice constant *a* is calculated as,

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

Chapter 3, Problem 27

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

Chapter 3, Solution 27

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,

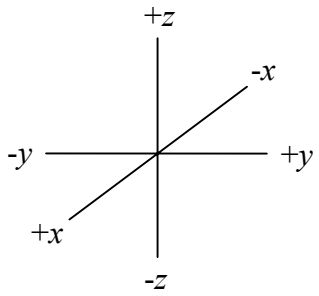
$$\text{HCP unit cell volume} = \frac{0.0618 \text{ nm}^3}{0.74} = \mathbf{0.084\ nm^3}$$

Chapter 3, Problem 28

How are atomic positions located in cubic unit cells?

Chapter 3, Solution 28

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 29

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

Chapter 3, Solution 29

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 30

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

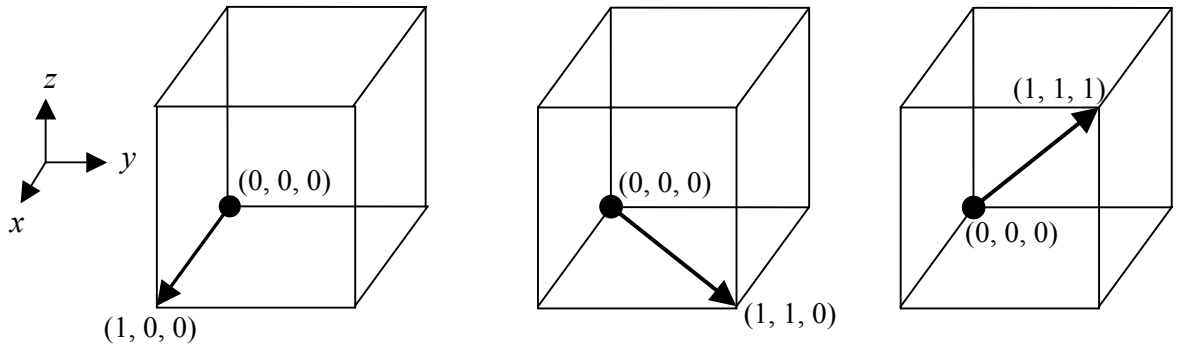
Chapter 3, Solution 30

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 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)

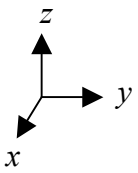
(c) Position Coordinates: (0, 0, 0), (1, 1, 1)

Chapter 3, Problem 32

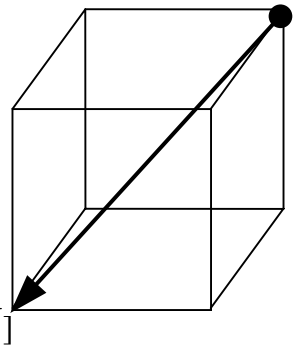
Draw direction vectors in unit cells for the following cubic directions:

(*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



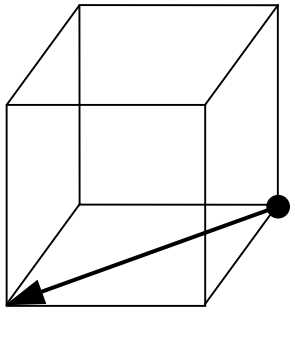
(a)



$x = +1$
$y = -1$
$z = -1$

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

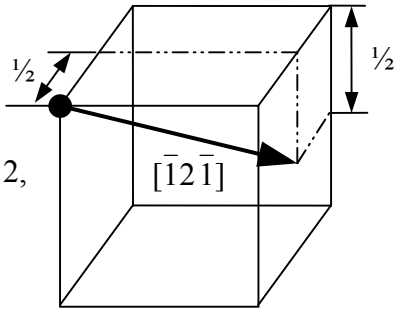
(b)



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

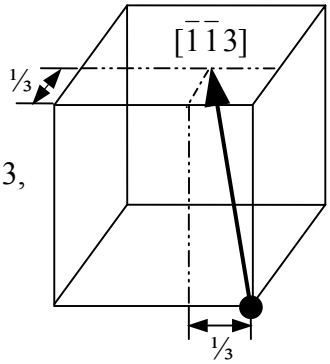
$[1\,\bar{1}\,0]$

(c)



Dividing by 2,
$x = -½$
$y = 1$
$z = -½$

(d)



Dividing by 3,
$x = -⅓$
$y = -⅓$
$z = 1$

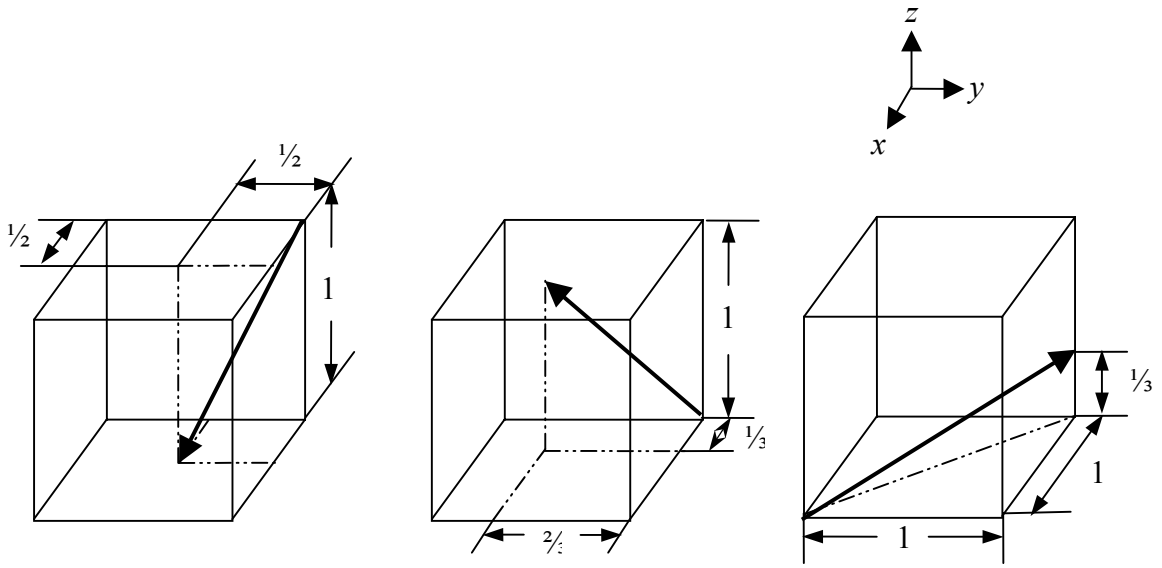
Chapter 3, Problem 33

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*) $[\bar{2}\bar{2}3]$

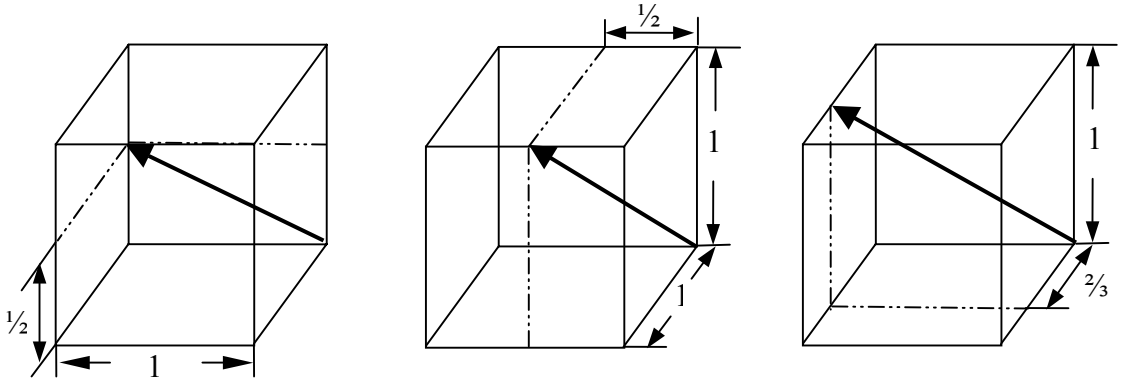
Chapter 3, Solution 33



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

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

$$\left(\frac{1}{4}, 1, \frac{1}{4} \right) \qquad [3\ 2\ 1]$$



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

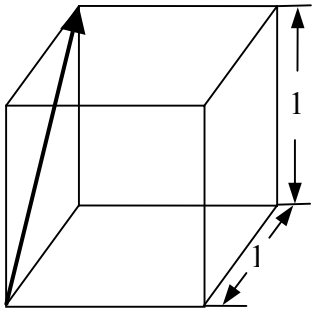
$$x = 0,\ y = -1,\ z = \frac{1}{2}$$

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

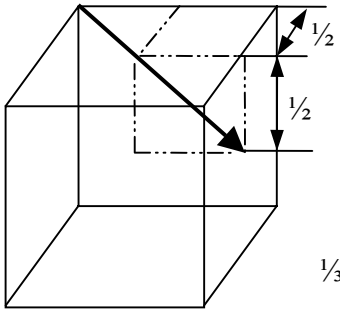
$$x = 1,\ y = -\frac{1}{2},\ z = 1$$

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

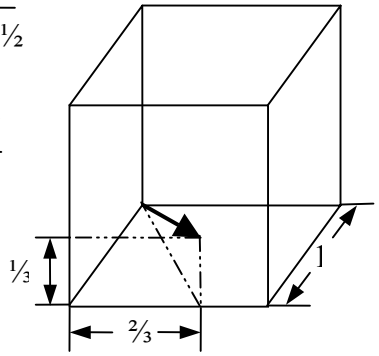
$$x = \frac{2}{3},\ y = -1,\ z = 1$$



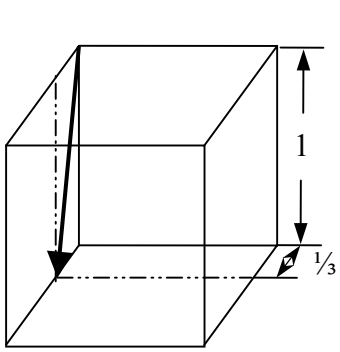
(g) For $[\bar{1}01]$,
$x=-1, y=0, z=1$



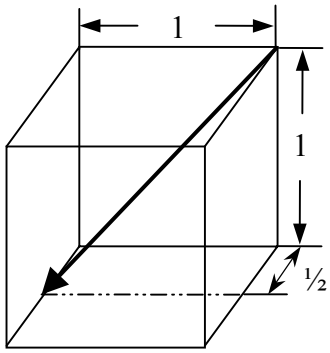
(h) Dividing $[12\bar{1}]$ by 2,
$x=\frac{1}{2}, y=1, z=-\frac{1}{2}$



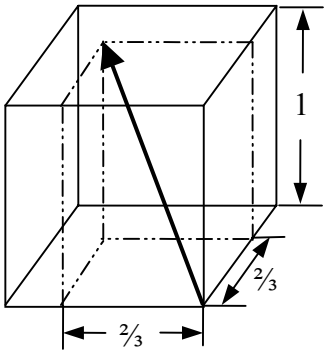
(i) Dividing [321] by 3,
$x=1, y=\frac{2}{3}, z=\frac{1}{3}$



(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?

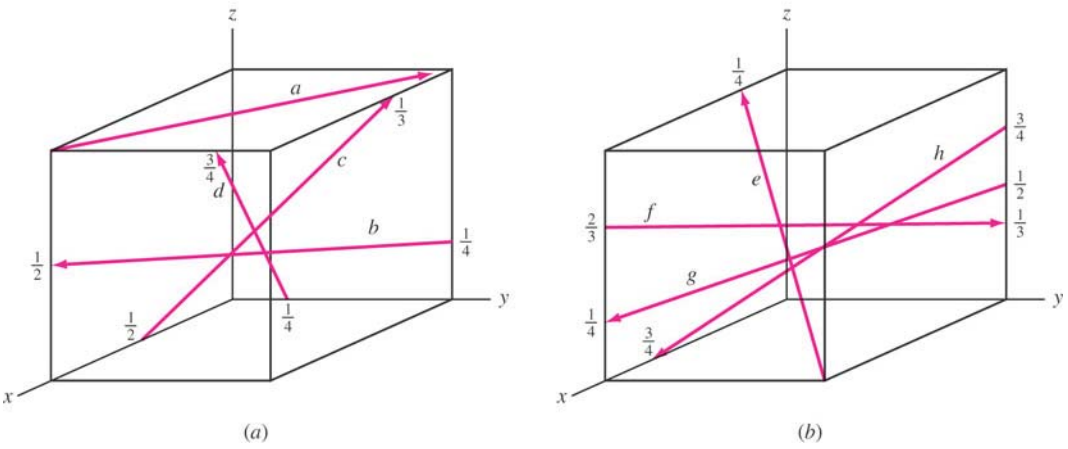
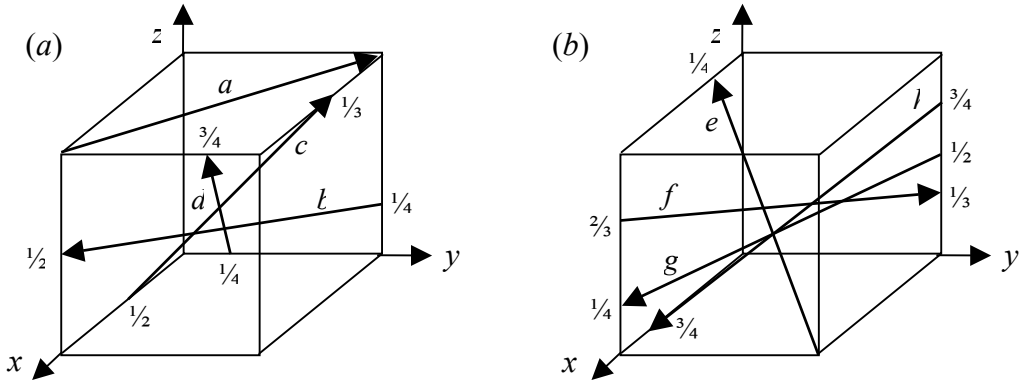
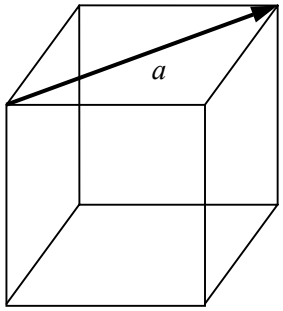


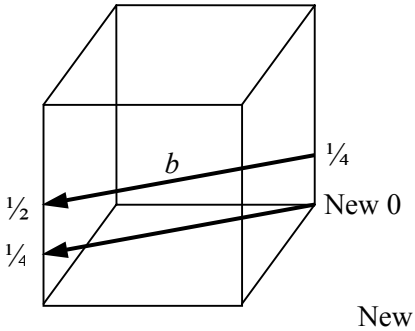
Figure P3.34

Chapter 3, Solution 34

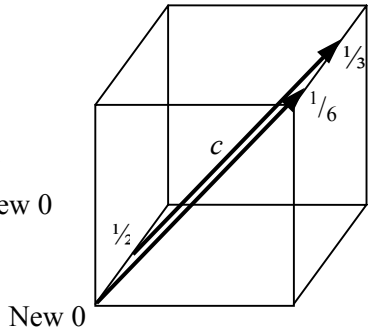




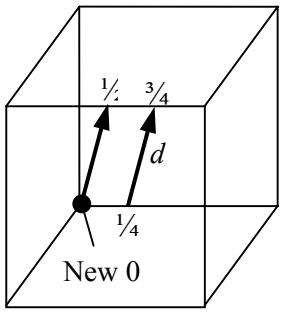
a. Vector components:
$x = -1,\ y = 1,\ z = 0$
Direction indices: $[\bar{1}10]$



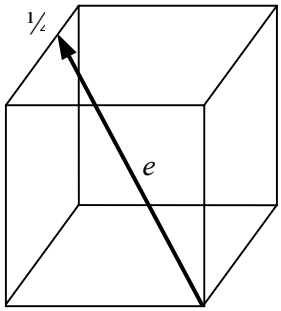
b. Moving direction vector down ¼ , vector components are: $x = 1,\ y = -1,\ z = ¼$
Direction indices: $[4\bar{4}1]$



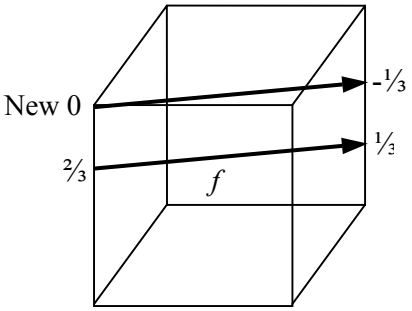
c. Moving direction vector forward ½, vector components are: $x = -1/6,\ y = 1,\ z = 1$
Direction indices: $[\bar{1}66]$



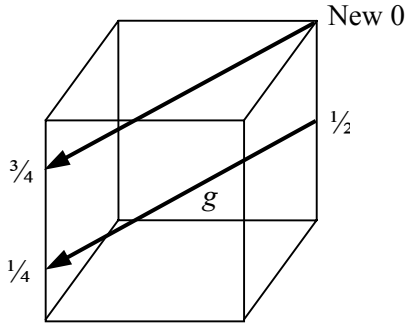
d. Moving direction vector left ¼, vector components are: $x = 1,\ y = ½,\ z = 1$
Direction indices: [212]



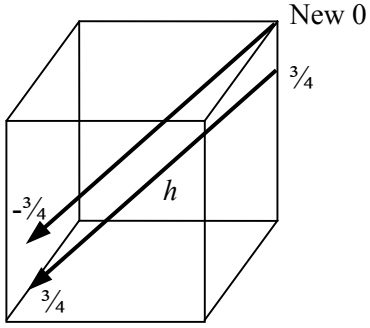
e. Vector components are:
$x = -¾,\ y = -1,\ z = 1$
Direction indices: $[\bar{3}\bar{4}4]$



f. Moving direction vector up ⅓, vector components are:
$x = -1,\ y = 1,\ z = -⅓$
Direction indices: $[\bar{3}31]$



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

Chapter 3, Solution 37

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 38

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

Chapter 3, Solution 38

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

Chapter 3, Problem 39

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

Chapter 3, Solution 39

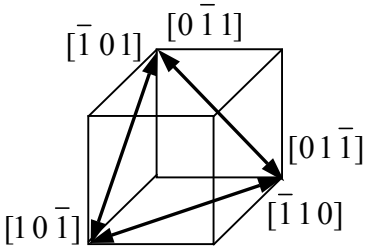
$$[111],\ [\bar{1}\bar{1}\bar{1}],\ [1\bar{1}1],\ [\bar{1}1\bar{1}],$$
$$[\bar{1}11],\ [1\bar{1}\bar{1}],\ [11\bar{1}],\ [\bar{1}\bar{1}1]$$

Chapter 3, Problem 40

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

Chapter 3, Solution 40

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

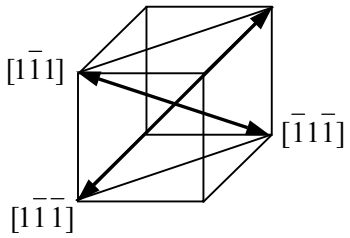


Chapter 3, Problem 41

What $\langle 1\,1\,1 \rangle$-type directions lie on the (110) plane of a cubic unit cell?

Chapter 3, Solution 41

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



Chapter 3, Problem 42

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 42

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.

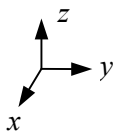
Chapter 3, Problem 43

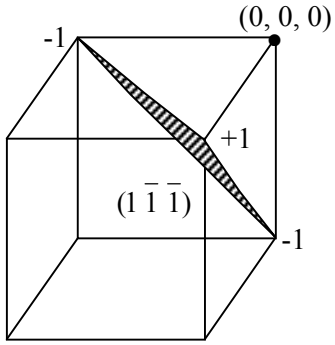
Draw in unit cubes the crystal planes that have the following Miller indices:

(*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*) $(3\,\bar{1}2)$

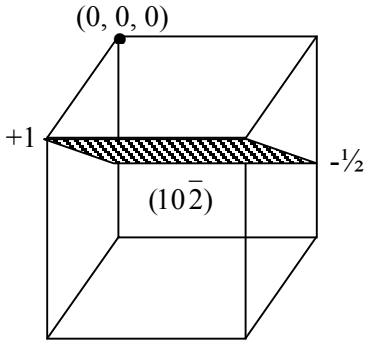
(*b*) $(10\bar{2})$ (*d*) $(21\bar{3})$ (*f*) $(30\bar{2})$ (*h*) $(\bar{2}1\bar{2})$ (*j*) $(13\bar{3})$ (*l*) $(\bar{3}3\,\bar{1})$

Chapter 3, Solution 43

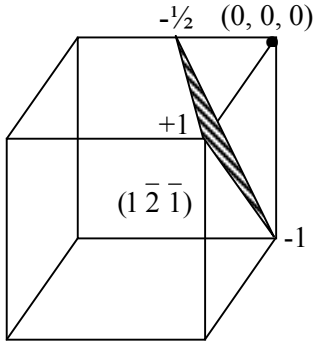




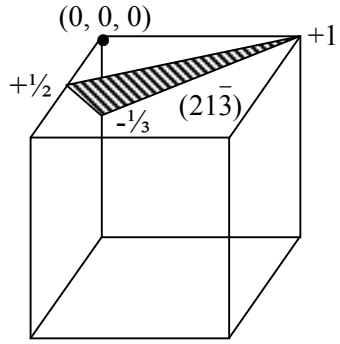
a. For $(1\,\bar{1}\,\bar{1})$ reciprocals are: $x = 1,\ y = -1,\ z = -1$



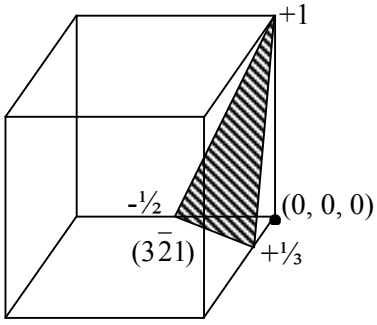
b. For $(10\bar{2})$ reciprocals are: $x = 1,\ y = \infty,\ z = -½$



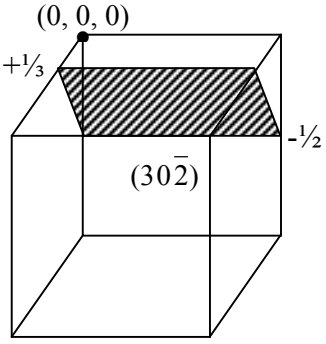
c. For $(1\,\bar{2}\,\bar{1})$ reciprocals are: $x = 1,\ y = -½,\ z = -1$



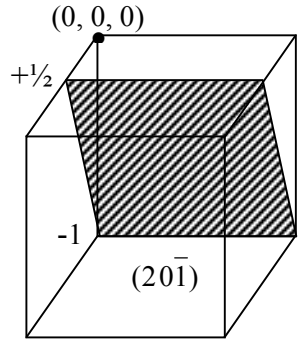
d. For $(21\bar{3})$ reciprocals are: $x = ½,\ y = 1,\ z = -⅓$



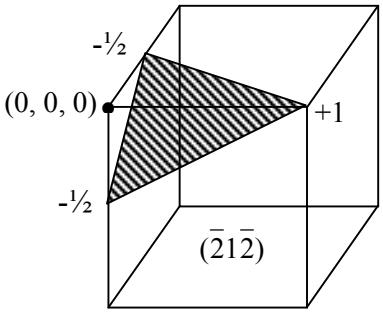
e. For $(3\bar{2}1)$ reciprocals are: $x = ⅓,\ y = -½,\ z = 1$



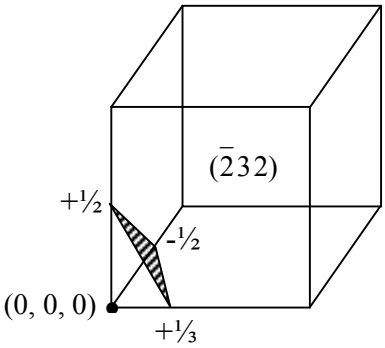
f. For $(30\bar{2})$ reciprocals are: $x = ⅓,\ y = \infty,\ z = -½$



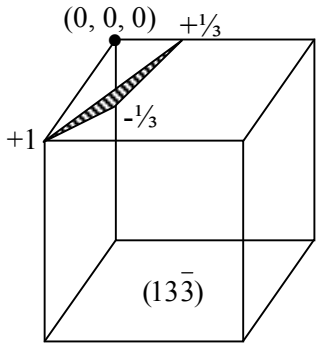
g. For $(20\bar{1})$ reciprocals are: $x = ½$, $y = \infty$, $z = -1$



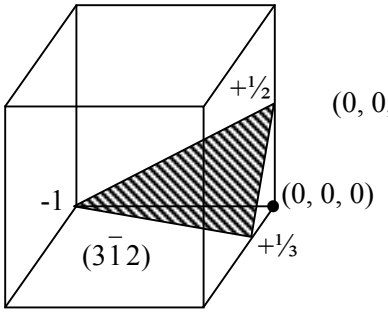
h. For $(\bar{2}1\bar{2})$ reciprocals are: $x = -½$, $y = 1$, $z = -½$



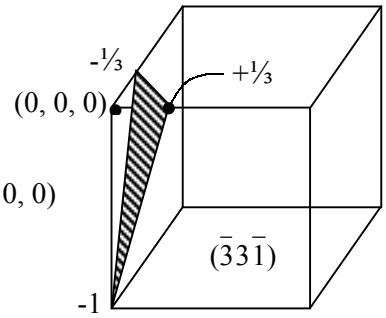
i. For $(\bar{2}32)$ reciprocals are: $x = -½$, $y = ⅓$, $z = ½$



j. For $(13\bar{3})$ reciprocals are: $x = 1$, $y = ⅓$, $z = -⅓$



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

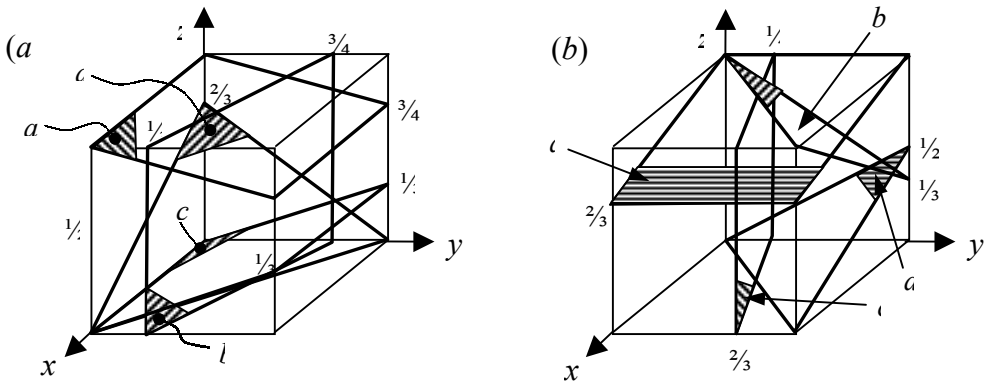


k. For $(\bar{3}3\bar{1})$ reciprocals are: $x = -⅓$, $y = ⅓$, $z = -1$

Chapter 3, Problem 44

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

Chapter 3, Solution 44



Miller Indices for Figure P3.44(a)

Plane *a* based on (0, 1, 1) as origin		**Plane *b* 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 **($\bar{5}$ $\bar{12}$ 0)**.	
Plane *c* based on (1, 1, 0) as origin		**Plane *d* 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 2 3)**.	

Miller Indices for Figure P3.44(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 $(1\ \bar{1}\ \bar{2})$.

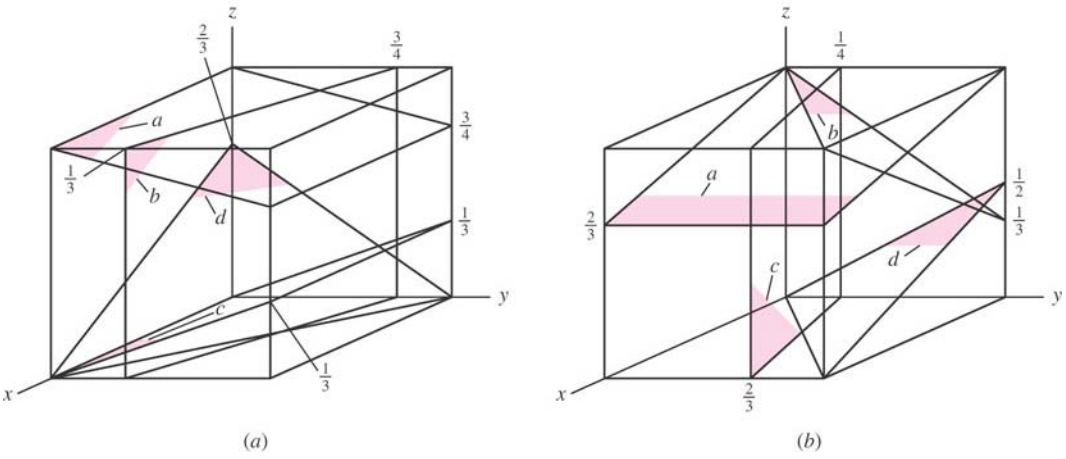


Figure P3.44

Chapter 3, Problem 45

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

Chapter 3, Solution 45

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

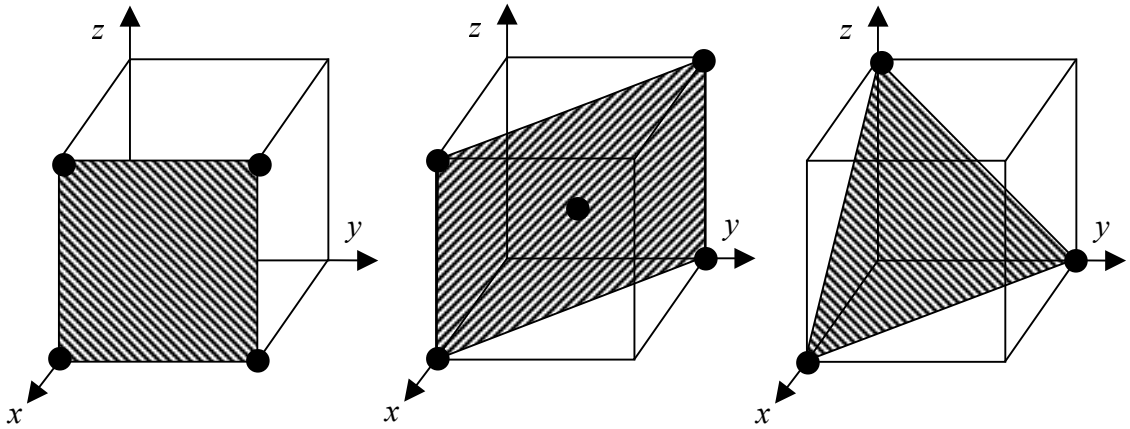
Chapter 3, Problem 46
What are the {100} family of planes of the cubic system?
Chapter 3, Solution 46

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

Chapter 3, Problem 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)

Chapter 3, Solution 47



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

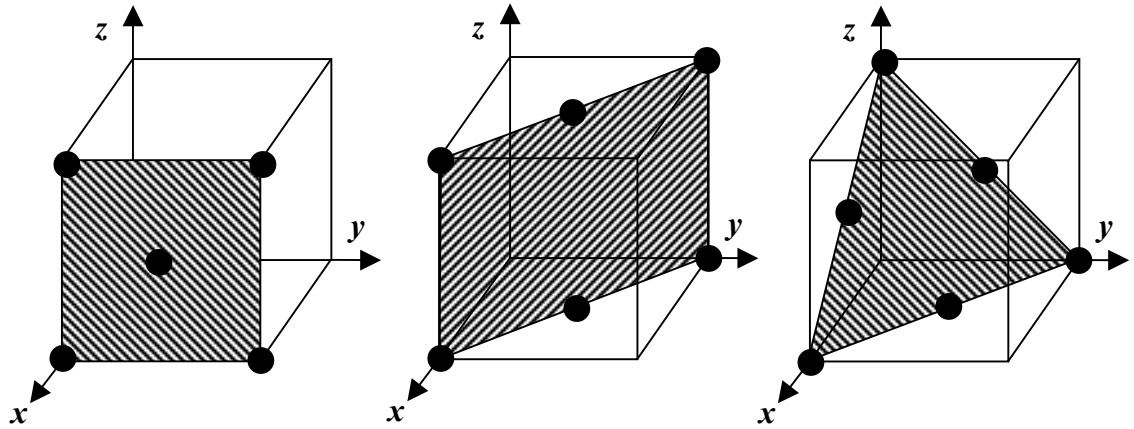
b. (1, 0, 0), (1, 0, 1), (0, 1, 0), (0, 1, 1), (½, ½, ½)

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

Chapter 3, Problem 48

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 48



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 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?

Chapter 3, Solution 49

Given the axial intercepts of (⅓, -⅔, ½), the reciprocal intercepts are: $\frac{1}{x} = 3,\quad \frac{1}{y} = -\frac{3}{2},\quad \frac{1}{z} = 2.$ Multiplying by 2 to clear the fraction, the Miller indices are $\mathbf{(6\,\bar{3}\,4)}$.

Chapter 3, Problem 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?

Chapter 3, Solution 50

Given the axial intercepts of (-½, -½, ⅔), the reciprocal intercepts are: $\frac{1}{x} = -2,\quad \frac{1}{y} = -2,\quad \frac{1}{z} = \frac{3}{2}.$ Multiplying by 2, the Miller indices are $\mathbf{(\bar{4}\,\bar{4}\,3)}$.

Chapter 3, Problem 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?

Chapter 3, Solution 51

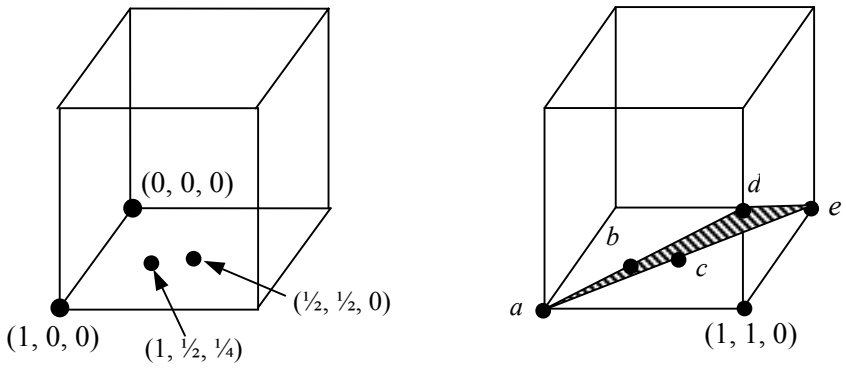
Given the axial intercepts of (1, ⅔, -½), the reciprocal intercepts are: $\frac{1}{x} = 1,\quad \frac{1}{y} = \frac{3}{2},\quad \frac{1}{z} = -2.$ Multiplying by 2, the Miller indices are $\mathbf{(2\ 3\ \bar{4})}$.

Chapter 3, Problem 52

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 52

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 $\mathbf{(\bar{1}\ \bar{1}\ 2)}$.

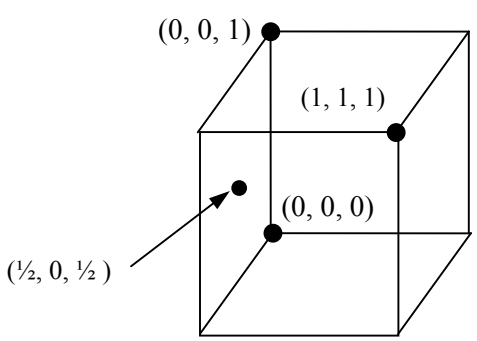


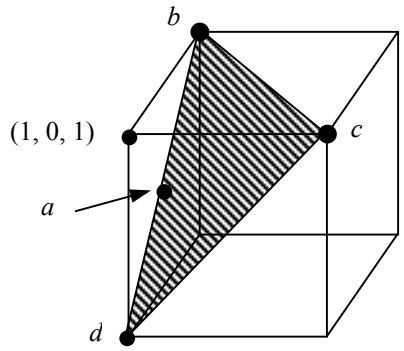
Chapter 3, Problem 53

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).

Chapter 3, Solution 53

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



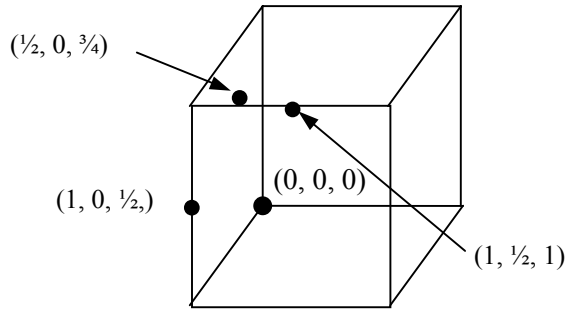


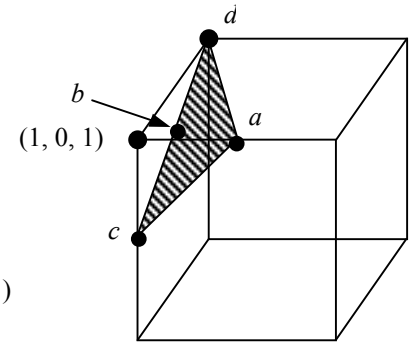
Chapter 3, Problem 54

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

Chapter 3, Solution 54

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





Chapter 3, Problem 55

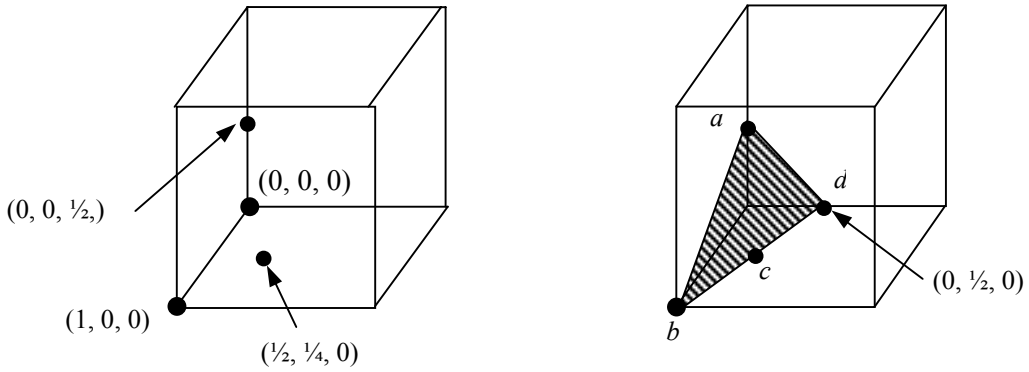
Determine the Miller indices of the cubic crystal plane that intersects the following position coordinates:
$(0,\ 0,\ \frac{1}{2});\ (1,0,0);\ (\frac{1}{2},\frac{1}{4},0)$.

Chapter 3, Solution 55

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 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}

Chapter 3, Solution 56

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

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

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

Chapter 3, Problem 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}

Chapter 3, Solution 57

(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 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?

Chapter 3, Solution 58

(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 59

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 58

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

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

Chapter 3, Problem 60

How are crystallographic planes indicated in HCP unit cells?

Chapter 3, Solution 60

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

Chapter 3, Problem 61

What notation is used to describe HCP crystal planes?

Chapter 3, Solution 61

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

Chapter 3, Problem 62

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

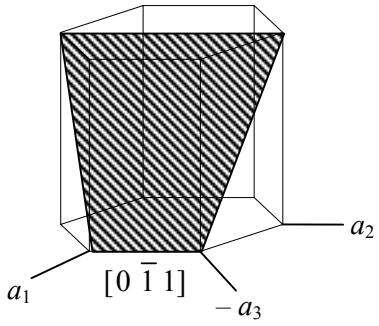
(*a*) $(10\bar{1}1)$ (*d*) $(1\bar{2}12)$ (*g*) $(\bar{1}2\bar{1}2)$ (*j*) $(\bar{1}100)$

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

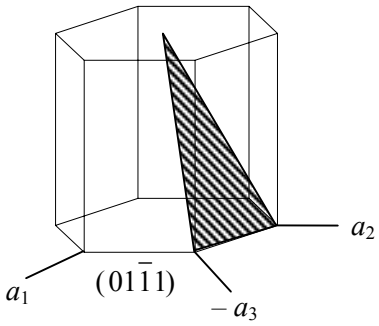
(*c*) $(\bar{1}2\bar{1}0)$ (*f*) $(1\bar{1}01)$ (*i*) $(10\bar{1}2)$ (*l*) $(\bar{1}012)$

Chapter 3, Solution 62

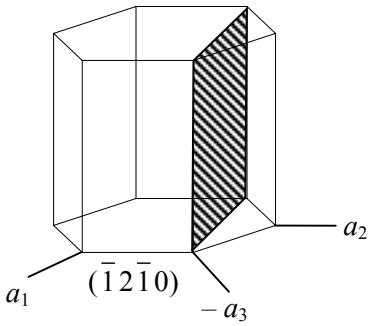
The reciprocals of the indices provided give the intercepts for the plane (a_1, a_2, a_3, and c).



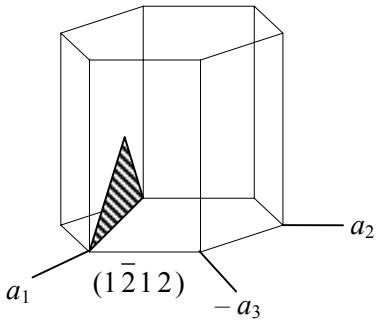
a. $a_1 = 1,\ a_2 = \infty,$
$a_3 = -1,\ c = 1$



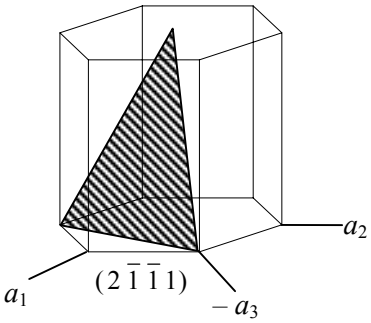
b. $a_1 = \infty,\ a_2 = 1,$
$a_3 = -1,\ c = 1$



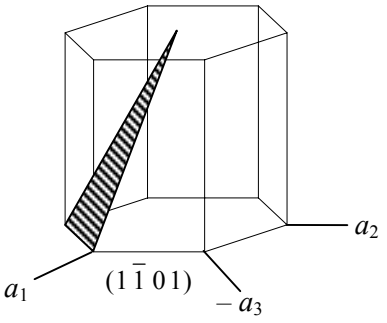
c. $a_1 = 1,\ a_2 = -\frac{1}{2},$
$a_3 = -1,\ c = \infty$



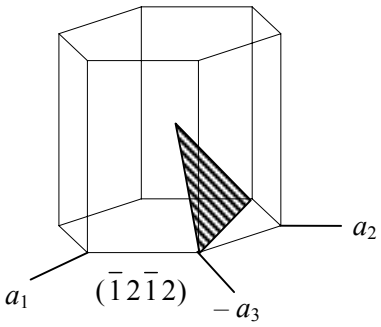
d. $a_1 = 1,\ a_2 = -\frac{1}{2},$
$a_3 = 1,\ c = \frac{1}{2}$



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

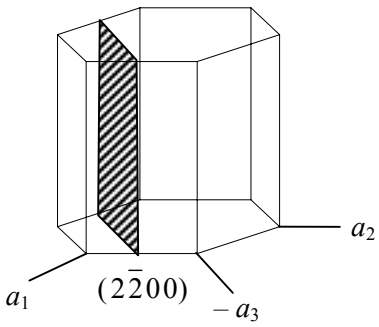


f. $a_1 = 1,\ a_2 = -1,$
$a_3 = \infty,\ c = 1$



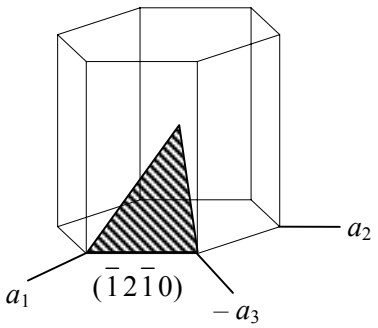
g. $a_1 = -1,\ a_2 = \dfrac{1}{2},$

$a_3 = -1,\ c = \dfrac{1}{2}$



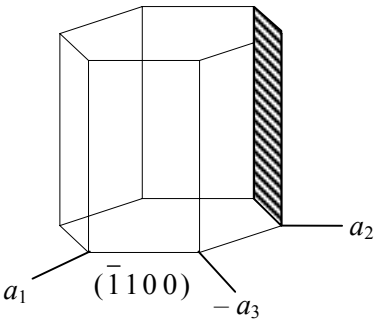
h. $a_1 = \dfrac{1}{2},\ a_2 = -\dfrac{1}{2},$

$a_3 = \infty,\ c = \infty$



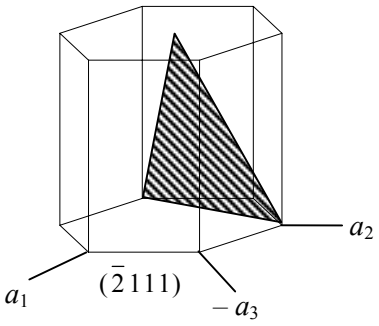
i. $a_1 = 1,\ a_2 = \infty,$

$a_3 = -1,\ c = \dfrac{1}{2}$



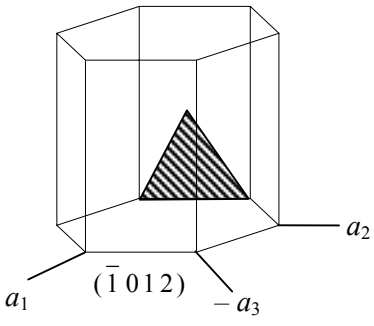
j. $a_1 = -1,\ a_2 = 1,$

$a_3 = \infty,\ c = \infty$



k. $a_1 = -\dfrac{1}{2},\ a_2 = 1,$

$a_3 = 1,\ c = 1$



l. $a_1 = -1,\ a_2 = \infty,$

$a_3 = 1,\ c = \dfrac{1}{2}$

Chapter 3, Problem 63

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

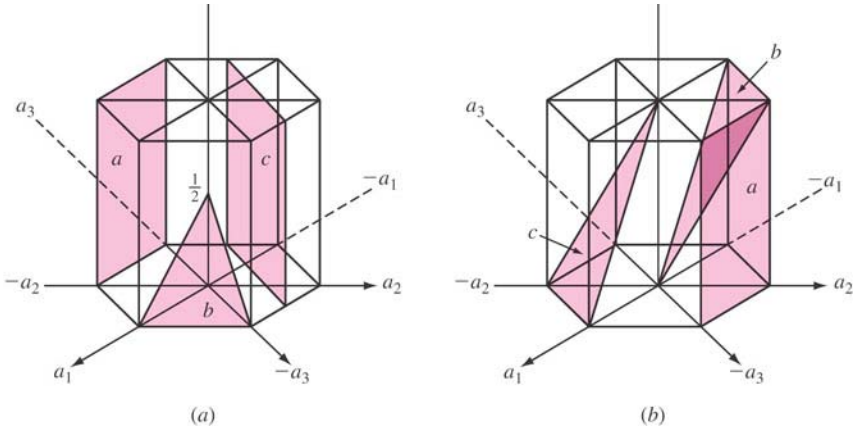


Figure P3.63

Chapter 3, Solution 63

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

Plane *a*		**Plane *b***		**Plane *c***	
Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts	Planar Intercepts	Reciprocals of Intercepts
$a_1 = \infty$	$\frac{1}{a_1} = 0$	$a_1 = 1$	$\frac{1}{a_1} = 1$	$a_1 = -½$	$\frac{1}{a_1} = -2$
$a_2 = -1$	$\frac{1}{a_2} = -1$	$a_2 = \infty$	$\frac{1}{a_2} = 0$	$a_2 = ½$	$\frac{1}{a_2} = 2$
$a_3 = 1$	$\frac{1}{a_3} = 1$	$a_3 = -1$	$\frac{1}{a_3} = -1$	$a_3 = \infty$	$\frac{1}{a_3} = 0$
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 $\mathbf{(0\ \bar{1}\ 1\ 0)}$.		The Miller indices of plane *b* are $\mathbf{(1\ 0\ \bar{1}\ 2)}$.		The Miller indices of plane *c* are $\mathbf{(\bar{2}\ 2\ 0\ 0)}$.	

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
$a_1 = \infty$	$\frac{1}{a_1} = 0$	$a_1 = 1$	$\frac{1}{a_1} = 1$	$a_1 = 1$	$\frac{1}{a_1} = 1$
$a_2 = 1$	$\frac{1}{a_2} = 1$	$a_2 = -1$	$\frac{1}{a_2} = -1$	$a_2 = -1$	$\frac{1}{a_2} = -1$
$a_3 = -1$	$\frac{1}{a_3} = -1$	$a_3 = \infty$	$\frac{1}{a_3} = 0$	$a_3 = \infty$	$\frac{1}{a_3} = 0$
$c = \infty$	$\frac{1}{c} = 0$	$c = 1$	$\left(\frac{1}{2}, 1, 0\right)$	$c = 1$	$\frac{1}{c} = 1$
The Miller indices of plane *a* are $\mathbf{(0\ 1\ \bar{1}\ 0)}$.		The Miller indices of plane *b* are $\mathbf{(1\ \bar{1}\ 0\ 1)}$.		The Miller indices of plane *c* are $\mathbf{(1\ \bar{1}\ 0\ 1)}$.	

Chapter 3, Problem 64

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

Chapter 3, Solution 64

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 65

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. 3.18*d*.

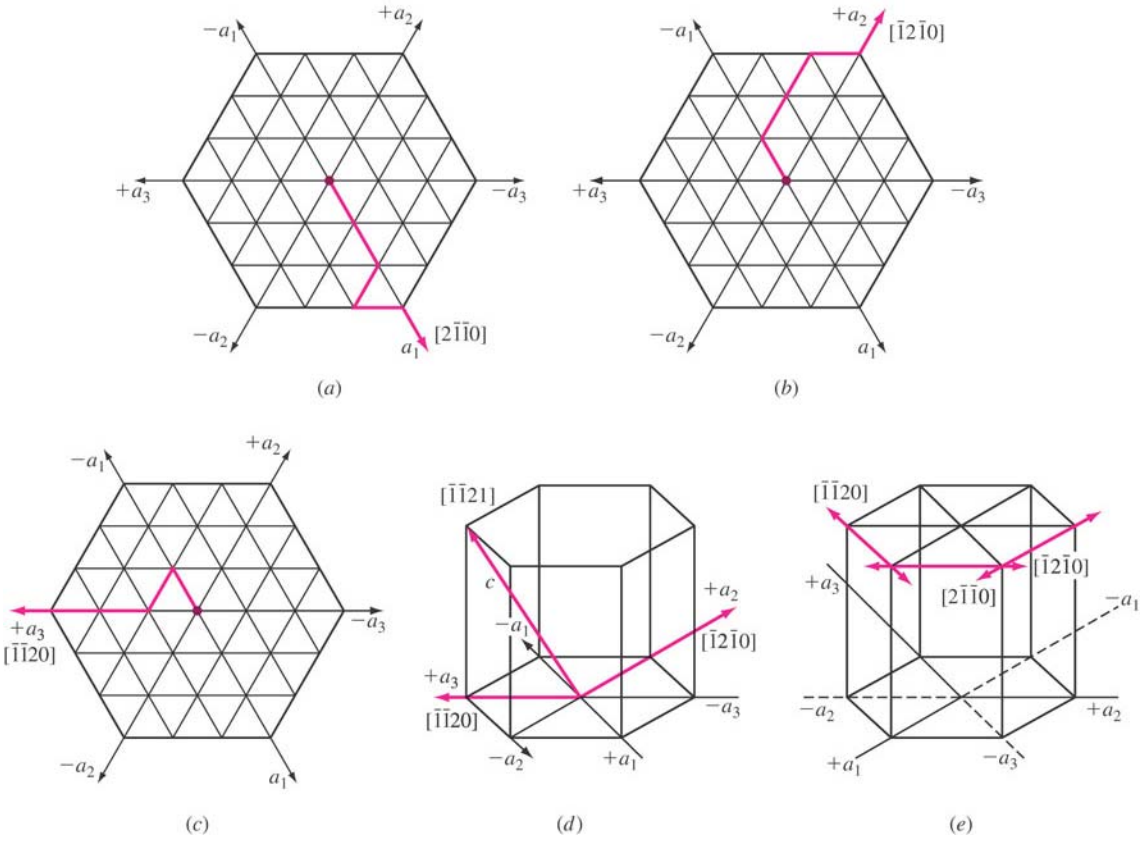
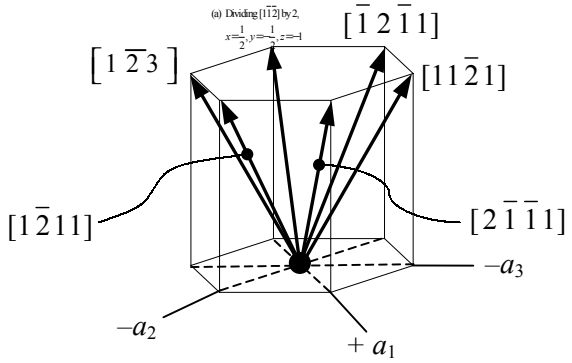


Figure 3.18

Chapter 3, Solution 65

$[\bar{1}\,\bar{1}\,2\,1], [\bar{2}\,1\,1\,1], [\bar{1}\,2\,\bar{1}\,1],$
$[1\,1\,\bar{2}\,1], [2\,\bar{1}\,\bar{1}\,1], [1\,\bar{2}\,1\,1]$

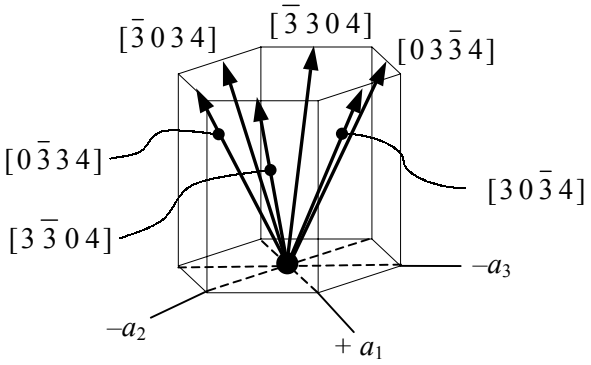


Chapter 3, Problem 66

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

Chapter 3, Solution 66

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



Chapter 3, Problem 67

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

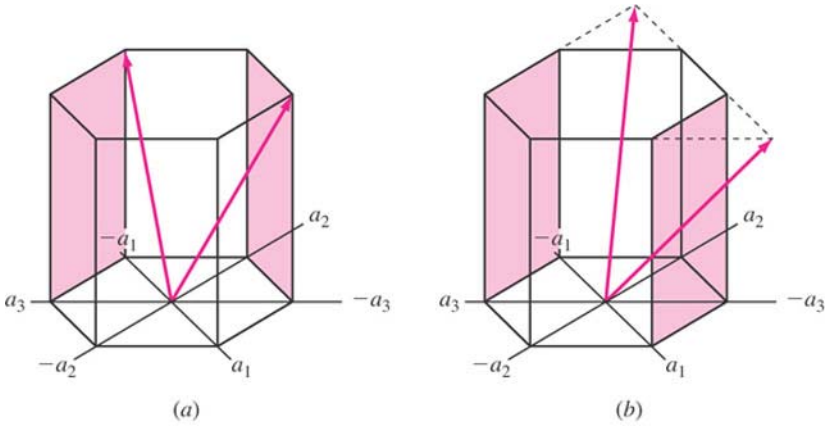
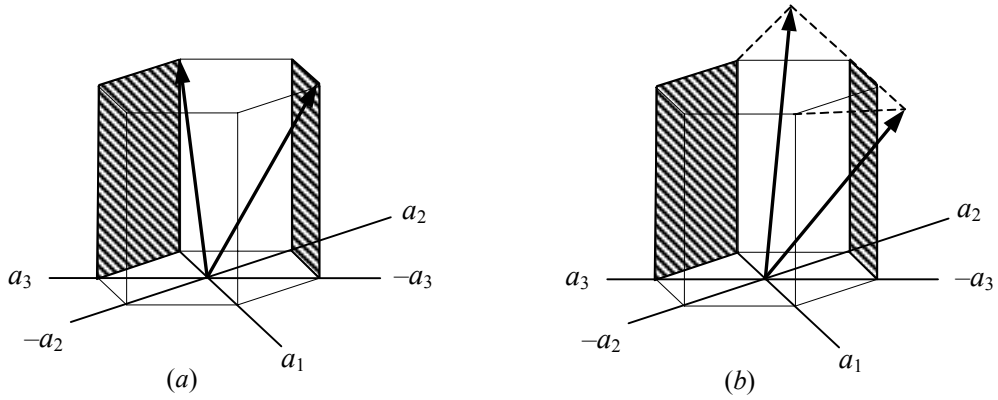


Figure P3.67

Chapter 3, Solution 67



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

Chapter 3, Problem 68

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

Chapter 3, Solution 68

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 69

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

Chapter 3, Solution 69

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

Chapter 3, Problem 70

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

Chapter 3, Solution 70

(a) The closest-packed directions in the FCC lattice are the $\langle \mathbf{1\,\bar{1}\,0} \rangle$ directions.

(b) The closest-packed directions in the HCP lattice are the $\langle \mathbf{1\,1\,\bar{2}\,0} \rangle$ directions.

Chapter 3, Problem 71

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 atomic mass.

Chapter 3, Solution 71

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

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

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

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

Chapter 3, Problem 72

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

Chapter 3, Solution 72

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,

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

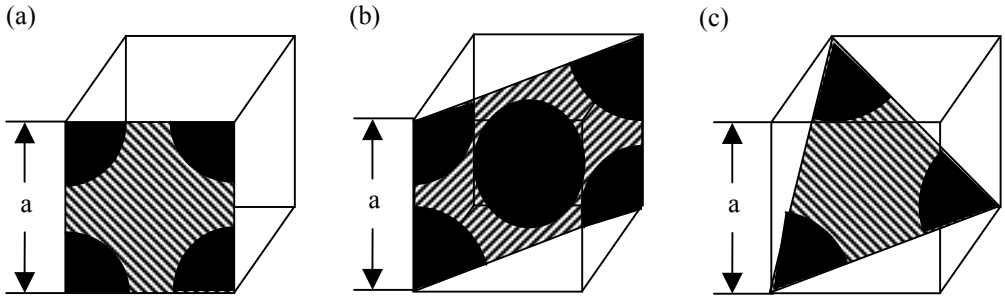
$$= 21,445,113\ \text{g/m}^3\left(\frac{\text{m}}{100\ \text{cm}}\right)^3 = \mathbf{21.45\ g/cm^3}$$

Chapter 3, Problem 73

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

Chapter 3, Solution 73

(Solution C is on the next page.)



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,

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

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

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

(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,

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

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

(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,

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

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

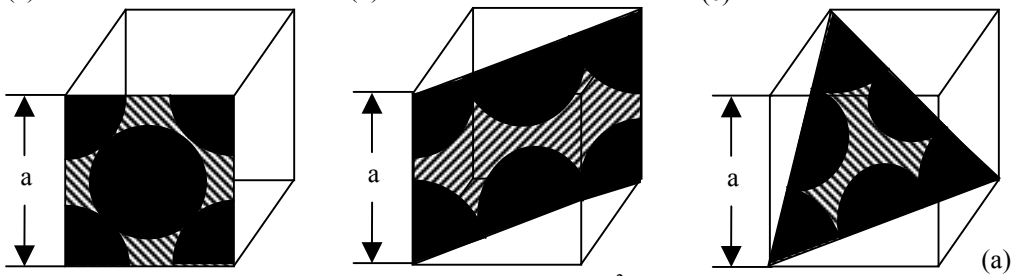
Chapter 3, Problem 74

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

Chapter 3, Solution 74

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

(a) (b) (c)



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

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

The density is therefore,

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

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

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

(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,

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

(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,

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

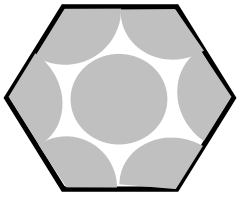
$$= \mathbf{1.963\times10^{13}\ atoms/mm^2}$$

Chapter 3, Problem 75

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 75

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,

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

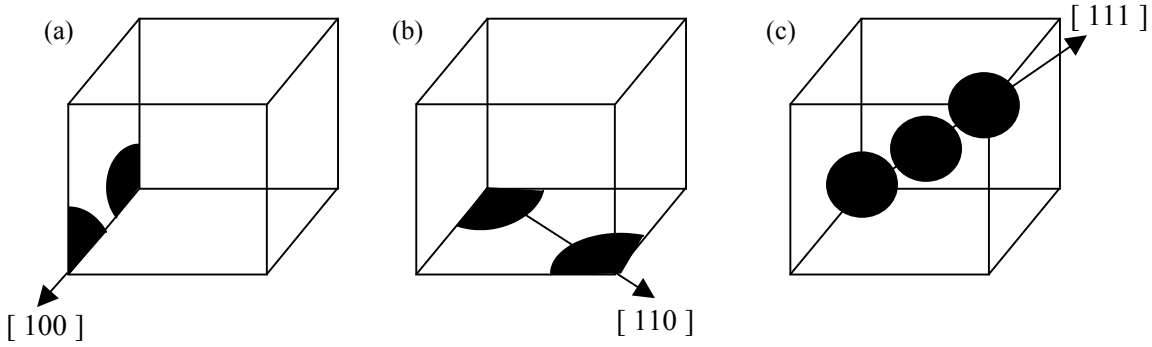
$$= \frac{3 \text{ atoms}}{\frac{3\sqrt{3}}{2}(0.22856 \times 10^{-9} \text{ m})^2} = (2.201 \times 10^{19} \text{atoms/m}^2)\left(\frac{\text{m}}{1000 \text{ mm}}\right)^2$$

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

Chapter 3, Problem 76

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

Chapter 3, Solution 76



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,

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

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

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

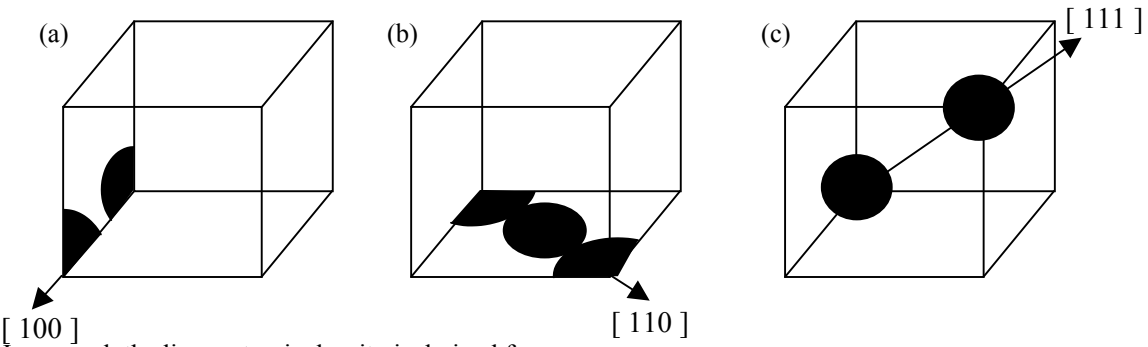
(c) For the [111] direction of BCC vanadium,

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

Chapter 3, Problem 77

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

Chapter 3, Solution 77



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 78

What is polymorphism with respect to metals?

Chapter 3, Solution 78

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 79

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 79

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

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

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

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

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 80

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 80

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 81

What are X rays, and how are they produced?

Chapter 3, Solution 81

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 82

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

Chapter 3, Solution 82

See Figure 3.25 of textbook.

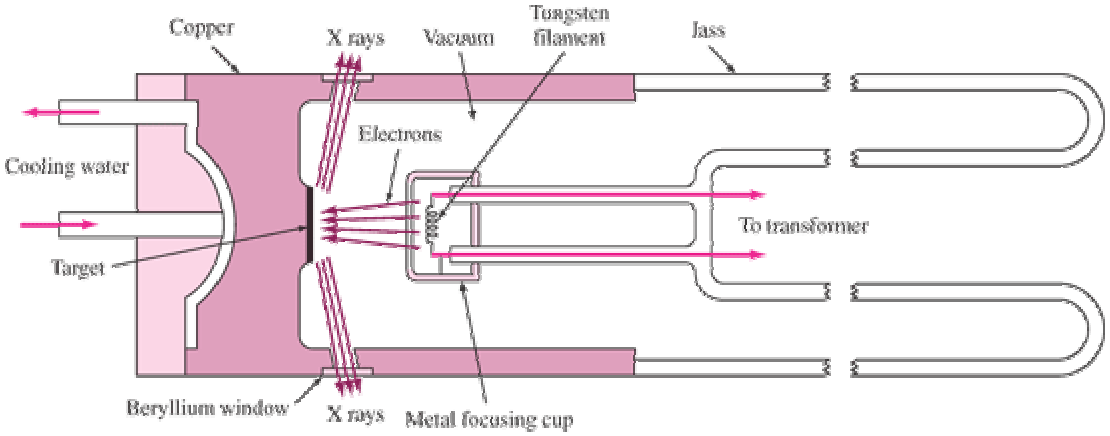


Figure 3.25

Chapter 3, Problem 83

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

Chapter 3, Solution 83

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 84

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

Chapter 3, Solution 84

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.

Chapter 3, Problem 85

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 85

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

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

Moreover, the *MP* and *PN* distances must equal $d_{hkl} \sin\theta$, where d_{hkl} is the crystal 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 86

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

Chapter 3, Solution 86

The interplanar distance is,

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

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 87

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 87

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,

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

Chapter 3, Problem 88

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 88

(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

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

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

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

(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 89

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 89

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

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

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

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

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

(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 90

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 90

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

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

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

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

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

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

Chapter 3, Problem 91

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 91

(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.