Chapter 1

Problem Solutions

1.1

(a) fcc: 8 corner atoms $\times 1/8 = 1$ atom
6 face atoms $\times 1/2 = 3$ atoms
Total of 4 atoms per unit cell

(b) bcc: 8 corner atoms $\times 1/8 = 1$ atom
1 enclosed atom $= 1$ atom
Total of 2 atoms per unit cell

(c) Diamond: 8 corner atoms $\times 1/8 = 1$ atom
6 face atoms $\times 1/2 = 3$ atoms
4 enclosed atoms $= 4$ atoms
Total of 8 atoms per unit cell

1.2

(a) Simple cubic lattice: $a = 2r$

Unit cell vol $= a^3 = (2r)^3 = 8r^3$

1 atom per cell, so atom vol $= (1)\left(\dfrac{4\pi r^3}{3}\right)$

Then

$$\text{Ratio} = \frac{\left(\dfrac{4\pi r^3}{3}\right)}{8r^3} \times 100\% = 52.4\%$$

(b) Face-centered cubic lattice

$$d = 4r = a\sqrt{2} \Rightarrow a = \frac{d}{\sqrt{2}} = 2\sqrt{2}\cdot r$$

Unit cell vol $= a^3 = \left(2\sqrt{2}\cdot r\right)^3 = 16\sqrt{2}\cdot r^3$

4 atoms per cell, so atom vol $= (4)\left(\dfrac{4\pi r^3}{3}\right)$

Then

$$\text{Ratio} = \frac{(4)\left(\dfrac{4\pi r^3}{3}\right)}{16\sqrt{2}\cdot r^3} \times 100\% = 74\%$$

(c) Body-centered cubic lattice

$$d = 4r = a\sqrt{3} \Rightarrow a = \frac{4}{\sqrt{3}}\cdot r$$

Unit cell vol $= a^3 = \left(\dfrac{4}{\sqrt{3}}\cdot r\right)^3$

2 atoms per cell, so atom vol $= (2)\left(\dfrac{4\pi r^3}{3}\right)$

Then

$$\text{Ratio} = \frac{(2)\left(\dfrac{4\pi r^3}{3}\right)}{\left(\dfrac{4r}{\sqrt{3}}\right)^3} \times 100\% = 68\%$$

(d) Diamond lattice

Body diagonal $= d = 8r = a\sqrt{3} \Rightarrow a = \dfrac{8}{\sqrt{3}}\cdot r$

Unit cell vol $= a^3 = \left(\dfrac{8r}{\sqrt{3}}\right)^3$

8 atoms per cell, so atom vol $= (8)\left(\dfrac{4\pi r^3}{3}\right)$

Then

$$\text{Ratio} = \frac{(8)\left(\dfrac{4\pi r^3}{3}\right)}{\left(\dfrac{8r}{\sqrt{3}}\right)^3} \times 100\% = 34\%$$

1.3

(a) $a = 5.43\ \mathring{A}$; From Problem 1.2d,

$$a = \frac{8}{\sqrt{3}}\cdot r$$

Then $r = \dfrac{a\sqrt{3}}{8} = \dfrac{(5.43)\sqrt{3}}{8} = 1.176\ \mathring{A}$

Center of one silicon atom to center of nearest neighbor $= 2r = 2.35\ \mathring{A}$

(b) Number density

$$= \frac{8}{\left(5.43\times 10^{-8}\right)^3} = 5\times 10^{22}\ \text{cm}^{-3}$$

(c) Mass density

$$= \rho = \frac{N(At.Wt.)}{N_A} = \frac{\left(5\times 10^{22}\right)(28.09)}{6.02\times 10^{23}}$$

$\Rightarrow \rho = 2.33$ grams/cm^3

1.4

(a) 4 Ga atoms per unit cell

$$\text{Number density } = \frac{4}{\left(5.65\times10^{-8}\right)^3}$$

$\Rightarrow$ Density of Ga atoms $= 2.22\times10^{22}$ cm^{-3}

4 As atoms per unit cell

$\Rightarrow$ Density of As atoms $= 2.22\times10^{22}$ cm^{-3}

(b) 8 Ge atoms per unit cell

$$\text{Number density } = \frac{8}{\left(5.65\times10^{-8}\right)^3}$$

$\Rightarrow$ Density of Ge atoms $= 4.44\times10^{22}$ cm^{-3}

1.5

From Figure 1.15

(a) $d = \left(\frac{a}{2}\right)\left(\frac{\sqrt{3}}{2}\right) = (0.4330)a$

$= (0.4330)(5.65) \Rightarrow d = 2.447\ \overset{o}{A}$

(b) $d = \left(\frac{a}{2}\right)\sqrt{2} = (0.7071)a$

$= (0.7071)(5.65) \Rightarrow d = 3.995\ \overset{o}{A}$

1.6

$$\sin\left(\frac{\theta}{2}\right) = \frac{\frac{a}{2}\sqrt{2}}{\frac{a}{2}\sqrt{3}} = \sqrt{\frac{2}{3}} \Rightarrow \frac{\theta}{2} = 54.74^\circ$$

$\Rightarrow \theta = 109.5^\circ$

1.7

(a) Simple cubic: $a = 2r = 3.9\ \overset{o}{A}$

(b) fcc: $a = \frac{4r}{\sqrt{2}} = 5.515\ \overset{o}{A}$

(c) bcc: $a = \frac{4r}{\sqrt{3}} = 4.503\ \overset{o}{A}$

(d) diamond: $a = \frac{2(4r)}{\sqrt{3}} = 9.007\ \overset{o}{A}$

1.8

(a) $2(1.035)\sqrt{2} = 2(1.035) + 2r_B$

$r_B = 0.4287\ \overset{o}{A}$

(b) $a = 2(1.035) = 2.07\ \overset{o}{A}$

(c) A-atoms: # of atoms $= 8\times\frac{1}{8} = 1$

$$\text{Density } = \frac{1}{\left(2.07\times10^{-8}\right)^3}$$

$= 1.13\times10^{23}$ cm^{-3}

B-atoms: # of atoms $= 6\times\frac{1}{2} = 3$

$$\text{Density } = \frac{3}{\left(2.07\times10^{-8}\right)^3}$$

$= 3.38\times10^{23}$ cm^{-3}

1.9

(a) $a = 2r = 4.5\ \overset{o}{A}$

# of atoms $= 8\times\frac{1}{8} = 1$

$$\text{Number density } = \frac{1}{\left(4.5\times10^{-8}\right)^3}$$

$= 1.097\times10^{22}$ cm^{-3}

$$\text{Mass density } = \rho = \frac{N(At.Wt.)}{N_A}$$

$$= \frac{\left(1.0974\times10^{22}\right)(12.5)}{6.02\times10^{23}}$$

$= 0.228$ gm/cm^3

(b) $a = \frac{4r}{\sqrt{3}} = 5.196\ \overset{o}{A}$

# of atoms $8\times\frac{1}{8}+1 = 2$

$$\text{Number density } = \frac{2}{\left(5.196\times10^{-8}\right)^3}$$

$= 1.4257\times10^{22}$ cm^{-3}

$$\text{Mass density } = \rho = \frac{\left(1.4257\times10^{22}\right)(12.5)}{6.02\times10^{23}}$$

$= 0.296$ gm/cm^3

1.10

From Problem 1.2, percent volume of fcc atoms is 74%; Therefore after coffee is ground,

Volume = 0.74 cm^3

1.11

(b) $a = 1.8 + 1.0 = 2.8\ \mathring{A}$

(c) Na: Density $= \dfrac{(1/2)}{(2.8\times10^{-8})^3}$

$= 2.28\times10^{22}\ \text{cm}^{-3}$

Cl: Density $= 2.28\times10^{22}\ \text{cm}^{-3}$

(d) Na: At. Wt. = 22.99
Cl: At. Wt. = 35.45

So, mass per unit cell

$$= \frac{\left(\frac{1}{2}\right)(22.99)+\left(\frac{1}{2}\right)(35.45)}{6.02\times10^{23}} = 4.85\times10^{-23}$$

Then mass density

$$\rho = \frac{4.85\times10^{-23}}{(2.8\times10^{-8})^3} = 2.21\ \text{grams/cm}^3$$

1.12

(a) $a\sqrt{3} = 2(2.2) + 2(1.8) = 8\ \mathring{A}$

Then $a = 4.62\ \mathring{A}$

Density of A:

$$= \frac{1}{(4.62\times10^{-8})^3} = 1.01\times10^{22}\ \text{cm}^{-3}$$

Density of B:

$$= \frac{1}{(4.62\times10^{-8})^3} = 1.01\times10^{22}\ \text{cm}^{-3}$$

(b) Same as (a)
(c) Same material

1.13

$$a = \frac{2(2.2)+2(1.8)}{\sqrt{3}} = 4.619\ \mathring{A}$$

(a) For 1.12(a), A-atoms

Surface density $= \dfrac{1}{a^2} = \dfrac{1}{(4.619\times10^{-8})^2}$

$= 4.687\times10^{14}\ \text{cm}^{-2}$

For 1.12(b), B-atoms: $a = 4.619\ \mathring{A}$

Surface density $= \dfrac{1}{a^2} = 4.687\times10^{14}\ \text{cm}^{-2}$

For 1.12(a) and (b), Same material

(b) For 1.12(a), A-atoms; $a = 4.619\ \mathring{A}$

Surface density

$$= \frac{1}{a^2\sqrt{2}} = 3.315\times10^{14}\ \text{cm}^{-2}$$

B-atoms;
Surface density

$$= \frac{1}{a^2\sqrt{2}} = 3.315\times10^{14}\ \text{cm}^{-2}$$

For 1.12(b), A-atoms; $a = 4.619\ \mathring{A}$

Surface density

$$= \frac{1}{a^2\sqrt{2}} = 3.315\times10^{14}\ \text{cm}^{-2}$$

B-atoms;
Surface density

$$= \frac{1}{a^2\sqrt{2}} = 3.315\times10^{14}\ \text{cm}^{-2}$$

For 1.12(a) and (b), Same material

1.14

(a) Vol. Density $= \dfrac{1}{a_o^3}$

Surface Density $= \dfrac{1}{a_o^2\sqrt{2}}$

(b) Same as (a)

1.15

(i) (110) plane
(see Figure 1.10(b))

(ii) (111) plane
(see Figure 1.10(c))

(iii) (220) plane $\Rightarrow \left(\frac{1}{2}, \frac{1}{2}, \infty\right) \Rightarrow (1,1,0)$

Same as (110) plane and [110] direction

(iv) (321) plane $\Rightarrow \left(\frac{1}{3}, \frac{1}{2}, \frac{1}{1}\right) \Rightarrow (2,3,6)$

Intercepts of plane at
$p = 2, q = 3, s = 6$

[321] direction is perpendicular to (321) plane

1.16

(a)

$$\left(\frac{1}{1},\frac{1}{3},\frac{1}{1}\right) \Rightarrow (313)$$

(b)

$$\left(\frac{1}{4},\frac{1}{2},\frac{1}{4}\right) \Rightarrow (121)$$

1.17

Intercepts: 2, 4, 3 $\Rightarrow \left(\frac{1}{2},\frac{1}{4},\frac{1}{3}\right) \Rightarrow$

(634) plane

1.18

(a) $d = a = 5.28 \overset{o}{A}$

(b) $d = \frac{a\sqrt{2}}{2} = 3.734 \overset{o}{A}$

(c) $d = \frac{a\sqrt{3}}{3} = 3.048 \overset{o}{A}$

1.19

(a) Simple cubic

(i) (100) plane:

$$\text{Surface density } = \frac{1}{a^2} = \frac{1}{\left(4.73\times10^{-8}\right)^2}$$
$$= 4.47\times10^{14}\text{ cm}^{-2}$$

(ii) (110) plane:

$$\text{Surface density } = \frac{1}{a^2\sqrt{2}}$$
$$= 3.16\times10^{14}\text{ cm}^{-2}$$

(iii) (111) plane:

$$\text{Area of plane } = \frac{1}{2}bh$$

where $b = a\sqrt{2} = 6.689 \overset{o}{A}$

Now

$$h^2 = \left(a\sqrt{2}\right)^2 - \left(\frac{a\sqrt{2}}{2}\right)^2 = \frac{3}{4}\left(a\sqrt{2}\right)^2$$

So $h = \frac{\sqrt{6}}{2}(4.73) = 5.793 \overset{o}{A}$

Area of plane

$$= \frac{1}{2}\left(6.68923\times10^{-8}\right)\left(5.79304\times10^{-8}\right)$$
$$= 19.3755\times10^{-16}\text{ cm}^2$$

$$\text{Surface density } = \frac{3\times\frac{1}{6}}{19.3755\times10^{-16}}$$
$$= 2.58\times10^{14}\text{ cm}^{-2}$$

(b) bcc

(i) (100) plane:

$$\text{Surface density } = \frac{1}{a^2} = 4.47\times10^{14}\text{ cm}^{-2}$$

(ii) (110) plane:

$$\text{Surface density } = \frac{2}{a^2\sqrt{2}}$$
$$= 6.32\times10^{14}\text{ cm}^{-2}$$

(iii) (111) plane:

$$\text{Surface density } = \frac{3\times\frac{1}{6}}{19.3755\times10^{-16}}$$
$$= 2.58\times10^{14}\text{ cm}^{-2}$$

(c) fcc

(i) (100) plane:

$$\text{Surface density } = \frac{2}{a^2} = 8.94\times10^{14}\text{ cm}^{-2}$$

(ii) (110) plane:

$$\text{Surface density } = \frac{2}{a^2\sqrt{2}}$$
$$= 6.32\times10^{14}\text{ cm}^{-2}$$

(iii) (111) plane:

$$\text{Surface density } = \frac{3\times\frac{1}{6}+3\times\frac{1}{2}}{19.3755\times10^{-16}}$$
$$= 1.03\times10^{15}\text{ cm}^{-2}$$

1.20

(a) (100) plane: - similar to a fcc:

$$\text{Surface density } = \frac{2}{\left(5.43\times10^{-8}\right)^2}$$
$$= 6.78\times10^{14}\text{ cm}^{-2}$$

(b) (110) plane:

$$\text{Surface density } = \frac{4}{\sqrt{2}\left(5.43\times10^{-8}\right)^2}$$
$$= 9.59\times10^{14}\text{ cm}^{-2}$$

(c) (111) plane:

Surface density $= \dfrac{2}{\left(\sqrt{3}/2\right)\left(5.43\times10^{-8}\right)^2}$
$= 7.83\times10^{14}\ \text{cm}^{-2}$

1.21

$$a = \frac{4r}{\sqrt{2}} = \frac{4(2.37)}{\sqrt{2}} = 6.703\ \overset{o}{A}$$

(a) $\#/\text{cm}^3 = \dfrac{8\times\frac{1}{8}+6\times\frac{1}{2}}{a^3} = \dfrac{4}{\left(6.703\times10^{-8}\right)^3}$
$= 1.328\times10^{22}\ \text{cm}^{-3}$

(b) $\#/\text{cm}^2 = \dfrac{4\times\frac{1}{4}+2\times\frac{1}{2}}{a^2\sqrt{2}}$
$= \dfrac{2}{\left(6.703\times10^{-8}\right)^2\sqrt{2}}$
$= 3.148\times10^{14}\ \text{cm}^{-2}$

(c) $d = \dfrac{a\sqrt{2}}{2} = \dfrac{(6.703)\sqrt{2}}{2} = 4.74\ \overset{o}{A}$

(d) # of atoms $= 3\times\dfrac{1}{6}+3\times\dfrac{1}{2} = 2$

Area of plane: (see Problem 1.19)

$$b = a\sqrt{2} = 9.4786\ \overset{o}{A}$$

$$h = \frac{\sqrt{6}a}{2} = 8.2099\ \overset{o}{A}$$

Area
$= \dfrac{1}{2}bh = \dfrac{1}{2}\left(9.4786\times10^{-8}\right)\left(8.2099\times10^{-8}\right)$
$= 3.8909\times10^{-15}\ \text{cm}^2$

$\#/\text{cm}^2 = \dfrac{2}{3.8909\times10^{-15}}$
$= 5.14\times10^{14}\ \text{cm}^{-2}$

$$d = \frac{a\sqrt{3}}{3} = \frac{(6.703)\sqrt{3}}{3} = 3.87\ \overset{o}{A}$$

1.22

Density of silicon atoms $= 5\times10^{22}\ \text{cm}^{-3}$ and 4 valence electrons per atom, so

Density of valence electrons $= 2\times10^{23}\ \text{cm}^{-3}$

1.23

Density of GaAs atoms
$= \dfrac{8}{\left(5.65\times10^{-8}\right)^3} = 4.44\times10^{22}\ \text{cm}^{-3}$

An average of 4 valence electrons per atom, So

Density of valence electrons
$= 1.77\times10^{23}\ \text{cm}^{-3}$

1.24

(a) $\dfrac{5\times10^{17}}{5\times10^{22}}\times100\% = 10^{-3}\%$

(b) $\dfrac{2\times10^{15}}{5\times10^{22}}\times100\% = 4\times10^{-6}\%$

1.25

(a) Fraction by weight
$\cong \dfrac{\left(2\times10^{16}\right)(10.82)}{\left(5\times10^{22}\right)(28.06)} = 1.542\times10^{-7}$

(b) Fraction by weight
$\cong \dfrac{\left(10^{18}\right)(30.98)}{\left(5\times10^{22}\right)(28.06)} = 2.208\times10^{-5}$

1.26

Volume density $= \dfrac{1}{d^3} = 2\times10^{16}\ \text{cm}^{-3}$

So $d = 3.684\times10^{-6}\ \text{cm} \Rightarrow d = 368.4\ \overset{o}{A}$

We have $a_o = 5.43\ \overset{o}{A}$

Then $\dfrac{d}{a_o} = \dfrac{368.4}{5.43} = 67.85$

1.27

Volume density $= \dfrac{1}{d^3} = 4\times10^{15}\ \text{cm}^{-3}$

So $d = 6.30\times10^{-6}\ \text{cm} \Rightarrow d = 630\ \overset{o}{A}$

We have $a_o = 5.43\ \overset{o}{A}$

Then $\dfrac{d}{a_o} = \dfrac{630}{5.43} = 116$