Fundamentals of Condensed Matter and Crystalline Physics

Instructor's Solution Manual

(rev. Dec. 2011)

CHAPTER 1

1-1. Show that the volume of the primitive cell of a BCC crystal lattice is $a^3/2$ where a is the lattice constant of the conventional cell.

1-1. Solution:

From Fig. 1.9, the primitive axes are

$$\vec{a}_1 = a\big((1/2)\hat{x} + (1/2)\hat{y} - (1/2)\hat{z}\big)$$
$$\vec{a}_2 = a\big((1/2)\hat{x} - (1/2)\hat{y} + (1/2)\hat{z}\big)$$
$$\vec{a}_3 = a\big(-(1/2)\hat{x} + (1/2)\hat{y} + (1/2)\hat{z}\big)$$

$$V = \left|(\vec{a}_1 \times \vec{a}_2)\cdot \vec{a}_3\right| = \left|\left(\frac{1}{2}\begin{vmatrix}\hat{x} & \hat{y} & \hat{z}\\ 1 & 1 & -1\\ 1 & -1 & 1\end{vmatrix}\right)\cdot \vec{a}_3\right| = a^3/2$$

1-2. Show that the volume of the primitive cell of a FCC crystal lattice is $a^3/4$ where a is the lattice constant of the conventional cell.

1-2. Solution:

From Fig. 1.9, the primitive axes are

$$\vec{a}_1 = a\big((1/2)\hat{x} + (1/2)\hat{y}\big)$$
$$\vec{a}_2 = a\big((1/2)\hat{x} + (1/2)\hat{z}\big)$$
$$\vec{a}_3 = a\big((1/2)\hat{y} + (1/2)\hat{z}\big)$$

$$V = \left|(\vec{a}_1 \times \vec{a}_2)\cdot \vec{a}_3\right| = \left|\left(\frac{1}{2}\begin{vmatrix}\hat{x} & \hat{y} & \hat{z}\\ 1 & 1 & 0\\ 1 & 0 & 1\end{vmatrix}\right)\cdot \vec{a}_3\right| = a^3/4$$

1-3. Show that the packing fraction of a BCC crystal lattice is $\sqrt{3}\pi/8 = 0.680$.

1-3. Solution:

From table 1-1, the nearest neighbor distance is $\sqrt{3}a/2$, and so the maximum radius of a balloon is $R = \sqrt{3}a/4$. There are a total of 2 balloons in each BCC unit cell for total occupied volume $\frac{8\pi}{3}R^3$ and packing fraction

$$\frac{8\pi R^3/3}{a^3} = \frac{8\pi(\sqrt{3}/4)^3}{3} = \frac{\sqrt{3}\pi}{8}$$

1-4. Show that the packing fraction of a FCC crystal lattice is $\sqrt{2}\pi/6 = 0.740$.

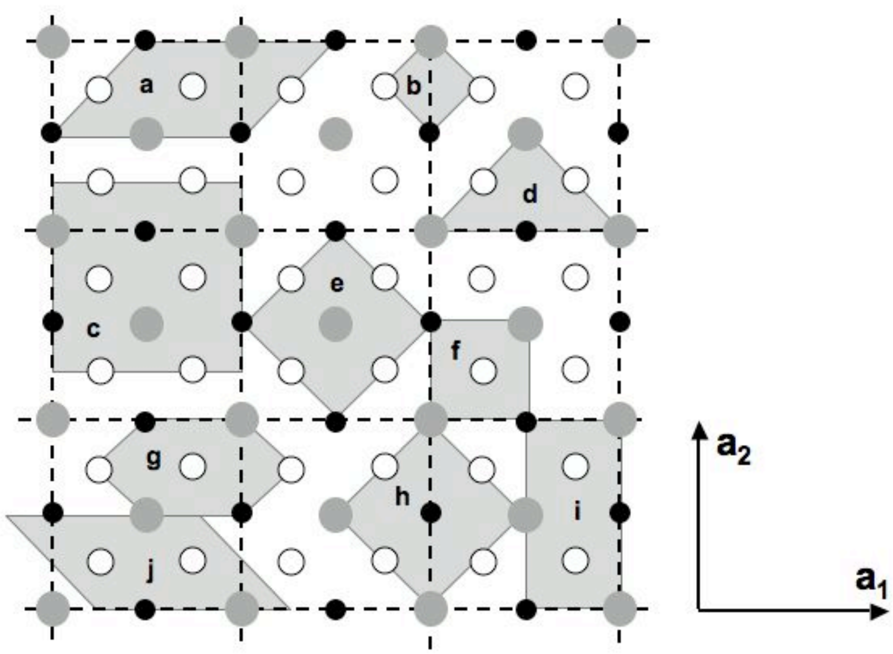
1-4. Solution:

From table 1-1, the nearest neighbor distance is $a/\sqrt{2}$, and so the maximum radius of a balloon is $R = a/2\sqrt{2}$. There are a total of 4 balloons in each BCC unit cell for total occupied volume $\frac{16\pi}{3}R^3$ and packing fraction

$$\frac{16\pi R^3/3}{a^3} = \frac{16\pi}{3}\left(\frac{1}{2\sqrt{2}}\right)^3 = \frac{\pi}{3\sqrt{2}} = \frac{\sqrt{2}\pi}{6}$$

1-5. The 2D crystal shown in Fig. 1-14 contains three atoms with a chemical formula ABC_2. Illustrated in the figure are several possible tiles. (a) Identify which of the tiles are primitive cells. (b) Identify which of the tiles are conventional cells. (c) Identify any tiles that are unable to correctly fill the space. (d) For each primitive cell, provide expressions for the appropriate basis vectors describing the basis set of atoms.

Fig. 1-14



1-5. Solution:

a) primitive cell with Black (0,0), Gray ((1/2),0), White (0, (1/2)), ((1/2),(1/2))
b) not primitive and will not tile space (note bad chemical formula)
c) conventional cell, will tile space
d) not primitive and will not tile space (note bad chemical formula)
e) primitive cell with Black ((1/2),0), Gray ((1/2),(1/2)), White ((1/4), (1/4)), ((3/4),(1/4))
f) not primitive and will not tile space (note bad chemical formula)
g) not primitive and will not tile space (note bad chemical formula)
h) primitive cell with Black (0,(1/2)), Gray (0,0), White ((1/4), (1/4)), ((1/4),(3/4))
i) primitive cell
j) primitive cell

1-6. Consider again the 2D crystal shown in Fig. 1-14. Describe all the basic symmetry operations (translational, rotational and mirror) satisfied by this lattice.

1-6. Solution:

Translational symmetry and 4-fold rotational symmetry. Mirror symmetry is found along any dashed line and any parallel line midway in between. Mirror symmetry is also found along any diagonal.

1-7. For the HCP crystal structure, show that the ideal *c/a* ratio is 1.633.

1-7. Solution:

Imagine balloons inflated about each site of the primitive cell shown in Fig. 1-12. The limitation arises from contact made in the half of the primitive cell containing a midpoint site. This half cell assumes the form of two tetrahedra (equilateral pyramids), one of which is inverted. Thus c/2 is the height of a pyramid of base a,

$\frac{c}{2} = a\sqrt{\frac{2}{3}}$ or $\frac{c}{a} = 2\sqrt{\frac{2}{3}} = 1.633$.

1-8. Bromine has an orthorhombic lattice structure with $|\vec{a}_1| = 4.65$ Å, $|\vec{a}_1| = 6.73$Å, $|\vec{a}_1| = 8.70$Å. (a) The atomic weight of bromine is 79.9 g/mol. If it has a density is 3.12 g/cc, how many bromine atoms reside in a single unit cell? (b) Which type of orthorhombic lattice (i.e, BC, FC etc.) is suggested your finding in part (a)? Explain. (c) If the atomic radius of bromine is 1.51Å, determine the packing fraction.

1-8. Solution:

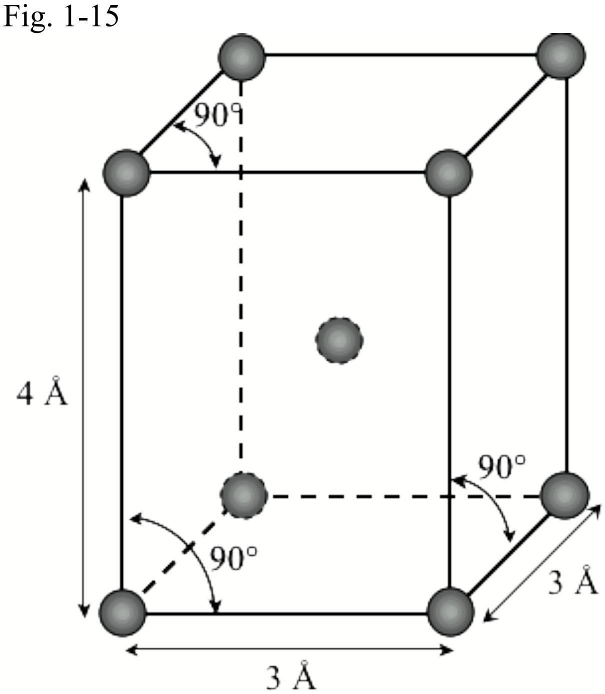
(a) $\rho = \frac{M}{V} = \frac{N(79.9/6.02x10^{23})}{(4.65x6.73x8.70)} \quad g/\mathring{A}^3 = 3.12\ g/cc \Rightarrow N \approx 8$

(b) Since bromine has a chemical formula of Br_2, there are 4 molecules of bromine in a unit cell, suggesting a FC orthorhombic structure.

(c) $$PF = \frac{8(4\pi(1.5)^3/3)}{(4.65x6.73x8.70)} = 0.333$$

1-9. Shown in Fig. 1-15 is the unit cell of a monatomic crystal. (a) How would you describe this particular crystal structure? (b) What is the maximum packing fraction you should expect for this specific structure?

Fig. 1-15



1-9. Solution:

(a) This unit cell has all 90° angles and two sides equal in length. From Fig. 1-7 we can identify it as tetragonal and, since there is a centered site inside, it would be referred to as body-centered tetragonal. (b) Imagine inflating balloons at each lattice site until contact is first made. One finds that the body diagonal is 5.831 Å and contact along this line would occur at an atom radius of r = 5.831/4 Å = 1.46 Å (just slightly shorter than half the distance in the base plane (1.50Å). The packing fraction is then

$$PF = \frac{2(4\pi(1.46)^3/3)}{(3x3x4)} = 0.724$$