8

Electronic Structure of Solids - Solutions

1. The cesium choride lattice is shown in Figure 8.5. Taking a lighter-shaded sphere to represent a cesium ion, we see that there are 8 chloride ions that serve as the nearest neighbors. Extrapolating the lines on Figure 8.5 in all directions, we see that there are two next-nearest neighbors along the axis for each of 3 dimensions, giving a total of 6 next-nearest neighbors for each cesium atom.

2. In Figure 8.6, a single cube of the face-centered cubic lattice is shown. Taking the original at the center of the bottom face of the cube, the four corners are generated for integer values of the primitive vectors $\mathbf{a} + \mathbf{b}$, where the distance a is from the center to a corner of the bottom square. Adding integer values of the primitive vector $\mathbf{c}$ give the upper four corners of the cube shown Figure 8.6. Hence these primitive vectors are an alternate way to describe the fcc lattice.

3. Referring to Fig. 8.8(b), we will use vectors to denote the locations of the carbon atoms from a fixed origin, then use vector relationships to determine the bond angle. First, select the origin to be located at point A in the lattice. The other two points of interest are point B and the atom located in the center of the top face shown. The primitive $\hat{\imath}$ and $\hat{\jmath}$ will be oriented along the edges of the top face (starting at point A) and the $\hat{k}$ vector will point directly upward from point A. We may now construct the position vectors to each point. Let $\mathbf{a}$ be the position vector from the origin to the top face-centered atom, while $\mathbf{b}$ points from point B to the origin (point A):

$$\mathbf{a} = \frac{1}{2}\hat{\imath} + \frac{1}{2}\hat{\jmath},\ \mathbf{b} = -\frac{1}{4}\hat{\imath} - \frac{1}{4}\hat{\jmath} + \frac{1}{4}\hat{k}$$

Our strategy will be to find the angle between $\mathbf{b}$ and $\mathbf{c}$. By inspection:

$$\mathbf{c} = \mathbf{a} + \mathbf{b}$$

Substituting the expressions for $\mathbf{a}$ and $\mathbf{b}$:

$$\mathbf{c} = \mathbf{a} + \mathbf{b} = \left(\frac{1}{2} - \frac{1}{4}\right)\hat{i} \ + \left(\frac{1}{2} - \frac{1}{4}\right)\hat{j} - \frac{1}{4}\hat{k}$$

$$= \frac{1}{4}\hat{i} + \frac{1}{4}\hat{j} - \frac{1}{4}\hat{k}$$

Now use the dot (or scalar) product of **b** and **c** to find the angle between the two:

$$\mathbf{b} \cdot \mathbf{c} = |\mathbf{b}||\mathbf{c}|cos(\theta)$$

For the left-hand side:

$$\mathbf{b} \cdot \mathbf{c} = -\frac{1}{16} - \frac{1}{16} + \frac{1}{16} = -\frac{1}{16}$$

For the right-hand side:

$$|\mathbf{b}||\mathbf{c}|cos(\theta) = \sqrt{\frac{3}{16}}\sqrt{\frac{3}{16}}cos(\theta) = \frac{3}{16}cos(\theta)$$

Equating the two:

$$-\frac{1}{16} = \frac{3}{16}cos(\theta)$$
$$cos(\theta) = -\frac{1}{3}$$
$$\theta = cos^{-1}\left(\frac{-1}{3}\right) = 109^\circ 28'$$

4. In a bcc lattice, as shown in Figure 8.3, the nearest neighbor is from the center to a corner of the cube. If a is the distance along an edge of the cube, then the distance from the center to the face of the cube is $a/2$. Using the Pythagorean formula, the distance from the center of the cube to the center of an edge is just $\sqrt{(a/2)^2 + (a/2)^2}$. Hence, the distance we want, from the center of the cube to a corner is

$$d = \sqrt{(a/2)^2 + (a/2)^2 + (a/2)^2} = \sqrt{3}(a/2)$$

5. For the simple cubic lattice, as shown in Figure 8.2, the nearest neighbor of any point will be located along the length of a side of the cube. Thus, the nearest neighbor distance is simply a. In the case of the fcc lattice, shown in Figure 8.6, the nearest neighbor distance is the midpoint distance along the diagonal of a face. Using the Pythagorean formula:

$$\sqrt{(a/2)^2 + (a/2)^2} = \sqrt{2}(a/2)$$

6. For sodium (Na) in a bcc crystal, with given density $\rho = 0.971\ g/cm^3$ and molar mass 23.0 g/mole, we want to find the lattice constant a. As shown in Figure 8.3, the bcc structure is made of two inter-spaced cubic lattices, each with lattice constant a. Each cube has unit volume a^3, giving a total of $n^3 = 2/a^3$ atoms per volume. Then the number of atoms per cm^3 is:

$$\frac{N}{V} = \frac{0.971\ g/cm^3}{23.0\ g/\text{mole}} \times (6.02 \times 10^{23}\ \text{atoms/mole}) = 2.54 \times 10^{22}\ cm^{-3}$$

Taking 1.0 cm^3 as the volume, $n^3 = 2.54 \times 10^{22}\ cm^{-3}$, so

$$\frac{1}{a} = (1.27 \times 10^{22})^{(1/3)}\ cm^{-1} = 2.33 \times 10^7\ cm^{-1}$$

Taking the reciprocal, $a = 4.3 \times 10^{-8}\ cm$. Hence, the nearest neighbor distance is:

$$\frac{\sqrt{3}}{2} a = 3.7 \times 10^{-8}\ cm = 3.7 \times 10^{-10}\ m$$

7. To find the center-to-center distance of the copper ions, first find the volume of one cell, which gives the length a, then use this to get the face-centered nearest-neighbor distance. The number of moles per unit volume for Cu is:

$$\frac{8.96\ g/cm^3}{63.5\ g/\text{mole}} = 0.141 \frac{\text{mole}}{cm^3}$$

and the number is:

$$0.141\ \frac{mole}{cm^3} \left(6.022 \times 10^{23}\ \frac{atoms}{mole}\right) = 8.494 \times 10^{22} \frac{atoms}{cm^3}$$

In section 8.2, just above Figure 8.7, it states that the face-centered cubic lattice has four atoms per cell:

$$\frac{4\ atoms/cell}{8.494 \times 10^{22}\ atoms/cm^3} = 4.709 \times 10^{-23}\ \frac{cm^3}{cell}$$

One edge of the cube has length:

$$a = (1.648 \times 10^{-22})^{1/3} = 3.611 \times 10^{-8}\ cm$$

From problem 5, the nearest-neighbor distance is then:

$$\frac{\sqrt{2}}{2} a = 2.553 \times 10^{-8}\ cm$$

8. Looking at Figure 8.6(b), the vectors to the center of the other faces can be written as:

$$v_1 = a\ \hat{i} + \frac{a}{2}(\hat{j} + \hat{k})$$
$$v_2 = a\ \hat{j} + \frac{a}{2}(\hat{k} + \hat{i})$$
$$v_3 = a\ \hat{k} + \frac{a}{2}(\hat{i} + \hat{j})$$

In terms of the primitive vectors:

$$\mathbf{a}_1 + \mathbf{a}_2 = \frac{a}{2}(\hat{j} + \hat{k}) + \frac{a}{2}(\hat{k} + \hat{i}) = v_3$$
$$\mathbf{a}_2 + \mathbf{a}_3 = \frac{a}{2}(\hat{k} + \hat{i}) + \frac{a}{2}(\hat{i} + \hat{j}) = v_1$$
$$\mathbf{a}_1 + \mathbf{a}_3 = \frac{a}{2}(\hat{j} + \hat{k}) + \frac{a}{2}(\hat{i} + \hat{j}) = v_2$$

9. Looking at Fig. 8.6(b), constructing the position vectors of each of the corners:

$$\mathbf{c}_1 = a\hat{k}$$
$$\mathbf{c}_2 = a\hat{j} + a\hat{k}$$
$$\mathbf{c}_3 = a\hat{i} + a\hat{j} + a\hat{k}$$
$$\mathbf{c}_4 = a\hat{i} + a\hat{k}$$

The primitive vectors from Eq. (8.4) are:

$$\mathbf{a}_1 = \frac{a}{2}\left(\hat{j} + \hat{k}\right),\ \mathbf{a}_2 = \frac{a}{2}\left(\hat{k} + \hat{i}\right),\ \mathbf{a}_3 = \frac{a}{2}\left(\hat{i} + \hat{j}\right)$$

Next, solve these primitive vectors for $\hat{i}, \hat{j}$, and $\hat{k}$. First add $\mathbf{a}_1$ and $\mathbf{a}_2$:

$$\mathbf{a}_1 + \mathbf{a}_2 = \frac{a}{2}\ (\hat{i} + \hat{j}) + a\hat{k}$$

Then subtract $\mathbf{a}_3$:

$$\mathbf{a}_1 + \mathbf{a}_2 - \mathbf{a}_3 = a\hat{k}$$

and solve for $\hat{k}$:

$$\hat{k} = \frac{\mathbf{a}_1 + \mathbf{a}_2 - \mathbf{a}_3}{a}$$

Similarly:

$$\hat{\imath} = \frac{\mathbf{a}_2 + \mathbf{a}_3 - \mathbf{a}_1}{a}$$

$$\hat{\jmath} = \frac{\mathbf{a}_1 - \mathbf{a}_2 + \mathbf{a}_3}{a}$$

Now substitute into the above:

$$\begin{aligned}
\mathbf{c}_1 &= \mathbf{a}_1 + \mathbf{a}_2 - \mathbf{a}_3 \\
\mathbf{c}_2 &= \mathbf{a}_1 - \mathbf{a}_2 + \mathbf{a}_3 + \mathbf{a}_1 + \mathbf{a}_2 - \mathbf{a}_3 = 2\mathbf{a}_1 \\
\mathbf{c}_3 &= \mathbf{a}_2 + \mathbf{a}_3 - \mathbf{a}_1 + \mathbf{a}_1 - \mathbf{a}_2 + \mathbf{a}_3 + \mathbf{a}_1 + \mathbf{a}_2 - \mathbf{a}_3 = \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3 \\
\mathbf{c}_4 &= \mathbf{a}_2 + \mathbf{a}_3 - \mathbf{a}_1 + \mathbf{a}_1 + \mathbf{a}_2 - \mathbf{a}_3 = 2\mathbf{a}_2
\end{aligned}$$

10. As above, the position vectors for the four upper corner in Fig. 8.4(b) are:

$$\begin{aligned}
\mathbf{c}_1 &= a\hat{k} \\
\mathbf{c}_2 &= a\hat{\jmath} + a\hat{k} \\
\mathbf{c}_3 &= a\hat{\imath} + a\hat{\jmath} + a\hat{k} \\
\mathbf{c}_4 &= a\hat{\imath} + a\hat{k}
\end{aligned}$$

The primitive vectors from Eq. (8.2) are:

$$\mathbf{a}_1 = \frac{a}{2}\left(\hat{\jmath} + \hat{k} - \hat{\imath}\right), \; \mathbf{a}_2 = \frac{a}{2}\left(\hat{k} + \hat{\imath} - \hat{\jmath}\right), \; \mathbf{a}_3 = \frac{a}{2}\left(\hat{\imath} + \hat{\jmath} - \hat{k}\right)$$

Following the same procedure as in Problem 9, the result is:

$$\begin{aligned}
\mathbf{c}_1 &= \mathbf{a}_1 + \mathbf{a}_2 \\
\mathbf{c}_2 &= \mathbf{a}_1 + 2\mathbf{a}_2 + \mathbf{a}_3 \\
\mathbf{c}_3 &= 2\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3 \\
\mathbf{c}_4 &= \mathbf{a}_1 + \mathbf{a}_2 + 2\mathbf{a}_3
\end{aligned}$$

11. Using the results from problems 4 and 5:

$$\begin{aligned}
\text{simplecubic} : d = a &\Rightarrow R = \frac{a}{2} \\
\text{bcc} : d = \frac{\sqrt{3}}{2}a &\Rightarrow R = \frac{\sqrt{3}}{4}a \\
\text{fcc} : d = \frac{2}{2}a &\Rightarrow R = \frac{\sqrt{2}}{4}a
\end{aligned}$$

substitute these values of R into the packing fraction equation:

$$\text{simple cubic} : F = (1)\frac{\frac{4}{3}\pi\left(\frac{a}{3}\right)^3}{a^3} = \frac{\pi}{6}$$
$$\text{bcc} : F = (2)\frac{\frac{4}{3}\pi\left(\frac{\sqrt{3}a}{4}\right)^3}{a^3} = \frac{\sqrt{3}\pi}{8}$$
$$\text{fcc} : F = (4)\frac{\frac{4}{3}\pi\left(\frac{\sqrt{2}a}{4}\right)^3}{a^3} = \frac{\sqrt{2}\pi}{6}$$

12. The goal is to prove Eq. (8.21),

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$$

where δ_{ij} is the Kronecker delta. Starting with $i = 1$ and $j = 1$:

$$\mathbf{b}_1 \cdot \mathbf{a}_1 = 2\pi\frac{a_1 \cdot (a_2 \times a_3)}{a_1 \cdot (a_2 \times a_3)} = 2\pi$$

and similarly for $i = j = 2$ and $i = j = 3$. Next consider $i = 1$ and $j = 2$:

$$\mathbf{b}_1 \cdot \mathbf{a}_2 = 2\pi\frac{a_2 \cdot (a_2 \times a_3)}{a_1 \cdot (a_2 \times a_3)}$$

and since $(a_2 \times a_3)$ is perpendicular to a_2, the numerator is zero. Similarly, for all $i \neq j$, the cross product in the numerator is perpendicular to the a_j vector, giving zero for the dot product. Hence Eq. (8.21) is correct.

13.

14.

15. The bcc primitive vectors are from Eq. (8.2):

$$\mathbf{a}_1 = \frac{a}{2}(\hat{j} + \hat{k} - \hat{i}) \text{ , } \mathbf{a}_2 = \frac{a}{2}(\hat{k} + \hat{i} \ - \hat{j}) \text{ , } \mathbf{a}_3 = \frac{a}{2}(\hat{i} + \hat{j} - \hat{k})$$

Use Eqs. (8.18)-(8.20) to calculate the primitive vectors of the bcc reciprocal lattice. But first do the cross-products:

$$\mathbf{a}_2 \times \mathbf{a}_3 = \frac{a^2}{4}\begin{vmatrix} \hat{\imath} & \hat{\jmath} & \hat{k} \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix} = \frac{a^2}{2}\hat{\jmath} + \frac{a^2}{2}\hat{k}$$

$$\mathbf{a}_3 \times \mathbf{a}_1 = \frac{a^2}{4}\begin{vmatrix} \hat{\imath} & \hat{\jmath} & \hat{k} \\ 1 & 1 & -1 \\ -1 & 1 & 1 \end{vmatrix} = \frac{a^2}{2}\hat{\imath} + \frac{a^2}{2}\hat{k}$$

$$\mathbf{a}_1 \times \mathbf{a}_2 = \frac{a^2}{4}\begin{vmatrix} \hat{\imath} & \hat{\jmath} & \hat{k} \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{vmatrix} = \frac{a^2}{2}\hat{\imath} + \frac{a^2}{2}\hat{\jmath}$$

Since the denominator of Eqs. (8.18)-(8.20) is the same, substitute it into each equation:

$$\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = \frac{a}{2}\left(\hat{\jmath} + \hat{k} - \hat{\imath}\right) \cdot \frac{a^2}{2}\left(\hat{\jmath} + \hat{k}\right) = \frac{a^3}{2}$$

Now use Eqs. (8.18)-(8.20) to get the primitive vectors of the reciprocal lattice:

$$\mathbf{b}_1 = 2\pi\left(\frac{2}{a^3}\right)\frac{a^2}{2}\left(\hat{\jmath} + \hat{k}\right) = \frac{2\pi}{a}\left(\hat{\jmath} + \hat{k}\right)$$
$$\mathbf{b}_2 = 2\pi\left(\frac{2}{a^3}\right)\frac{a^2}{2}\left(\hat{\imath} + \hat{k}\right) = \frac{2\pi}{a}\left(\hat{\imath} + \hat{k}\right)$$
$$\mathbf{b}_3 = 2\pi\left(\frac{2}{a^3}\right)\frac{a^2}{2}\left(\hat{\imath} + \hat{\jmath}\right) = \frac{2\pi}{a}\left(\hat{\imath} + \hat{\jmath}\right)$$

This bcc reciprocal lattice, when compared with Eq. (8.4), is just a fcc lattice with cell length $4\pi/a$.

16. Use Eqs. (8.18)-(8.20) to calculate the primitive vectors of the fcc reciprocal lattice. But, first do the cross-products:

$$\mathbf{a}_2 \times \mathbf{a}_3 = \frac{a^2}{4}\begin{vmatrix} \hat{\imath} & \hat{\jmath} & \hat{k} \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix} = \frac{a^2}{4}(-\hat{\imath} + \hat{\jmath} + \hat{k})$$

$$\mathbf{a}_3 \times \mathbf{a}_1 = \frac{a^2}{4}\begin{vmatrix} \hat{\imath} & \hat{\jmath} & \hat{k} \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{vmatrix} = \frac{a^2}{4}(\hat{\imath} - \hat{\jmath} + \hat{k})$$

$$\mathbf{a}_1 \times \mathbf{a}_2 = \frac{a^2}{4}\begin{vmatrix} \hat{\imath} & \hat{\jmath} & \hat{k} \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix} = \frac{a^2}{4}(\hat{\imath} + \hat{\jmath} - \hat{k})$$

The denominator of Eqs. (8.18)-(8.20) is the same for each vector:

$$\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = \frac{a}{2}\left(\hat{j} + \hat{k}\right) \cdot \frac{a^2}{4}\left(-\hat{i} + \hat{j} + \hat{k}\right) = \frac{a^3}{4}$$

Now use Eq. (8.18)-(8.20) to get the primitive vectors of the reciprocal lattice:

$$\begin{aligned} \mathbf{b}_1 &= \frac{2\pi}{a}\ \left(-\hat{i} + \hat{j} + \hat{k}\right) \\ \mathbf{b}_2 &= \frac{2\pi}{a}\ \left(\hat{i} - \hat{j} + \hat{k}\right) \\ \mathbf{b}_3 &= \frac{2\pi}{a}\ \left(\hat{i} + \hat{j} - \hat{k}\right) \end{aligned}$$

When compared with Eq. (8.2), this a bcc lattice with cell length $4\pi/a$.

17. Use Eqs. (8.18)-(8.20) to calculate the primitive vectors of the hexagonal close-packed reciprocal lattice. But, first do the cross-products:

$$\mathbf{b} \times \mathbf{c} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ -(\sqrt{3}a/2) & (a/2) & 0 \\ 0 & 0 & c \end{vmatrix} = \frac{ac}{2}(\hat{i} + \sqrt{3}\hat{j})$$

$$\mathbf{c} \times \mathbf{a} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 0 & 0 & c \\ (\sqrt{3}a/2) & (a/2) & 0 \end{vmatrix} = \frac{ac}{2}(-\hat{i} + \sqrt{3}\hat{j})$$

$$\mathbf{a} \times \mathbf{b} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ (\sqrt{3}a/2) & (a/2) & 0 \\ -(\sqrt{3}a/2) & (a/2) & 0 \end{vmatrix} = \frac{\sqrt{3}a^2}{2}(\hat{k})$$

The denominator of Eqs. (8.18)-(8.20) is the same for each vector:

$$\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \frac{a}{2}\left(\sqrt{3}\hat{i} + \hat{j}\right) \cdot \frac{ac}{2}\left(\hat{i} + \sqrt{3}\hat{j}\right) = \frac{\sqrt{3}a^2 c}{2}$$

Now use Eq. (8.18)-(8.20) to get the primitive vectors of the reciprocal lattice:

$$\begin{aligned} \mathbf{b}_1 &= \frac{2\pi}{\sqrt{3}a}\left(\hat{i} + \sqrt{3}\hat{j}\right) \\ \mathbf{b}_2 &= \frac{2\pi}{\sqrt{3}a}\left(-\hat{i} + \sqrt{3}\hat{j}\right) \\ \mathbf{b}_3 &= \frac{2\pi}{c}\ \left(\hat{k}\right) \end{aligned}$$

This is the same as the original lattice but with cell lengths $4\pi/(3a)$ in the x-y plane and $4\pi/c$ along the z axis. The volume of a unit cell is given by:

$$V = \mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3) = \frac{2\pi}{\sqrt{3}a}\left(\hat{\imath} + \sqrt{3}\hat{\jmath}\right) \cdot \frac{4\pi^2}{\sqrt{3}a^2}\left(\sqrt{3}\hat{\imath} + \hat{\jmath}\right) = \frac{16\pi^3}{\sqrt{3}a^3}$$

18. Following the equation just below Fig. 8.6, there must be some combination of primitive vectors that allow translation by one cell length along the z-axis:

$$a\hat{k} = \mathbf{a} + \mathbf{b} - \mathbf{c} = a\hat{\jmath} - \mathbf{c}$$

Hence, $\mathbf{c} = a(\hat{\jmath} - \hat{k})$ to allow translations along the z-axis.

19. Start with Eqs. (8.18)-(8.20) to show that:

$$\mathbf{a}_1 = 2\pi \frac{\mathbf{b}_2 \times \mathbf{b}_3}{\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3)} \qquad (1)$$

$$\mathbf{a}_2 = 2\pi \frac{\mathbf{b}_3 \times \mathbf{b}_1}{\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3)} \qquad (2)$$

$$\mathbf{a}_1 = 2\pi \frac{\mathbf{b}_1 \times \mathbf{b}_2}{\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3)} \qquad (3)$$

Where $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$ are given by Eqs. (8.18)-(8.20). First calculate the cross-product $\mathbf{b}_2 \times \mathbf{b}_3$ since it will be used in each equation.

$$\mathbf{b}_2 \times \mathbf{b}_3 = 4\pi^2 \left(\frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}\right) \times \left(\frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}\right)$$

Note that the denominators of the terms on each side of the cross-product are a scalar quantity. Therefore, it can be brought outside the vector product. Proceeding with the numerator:

$$(\mathbf{a}_3 \times \mathbf{a}_1) \times (\mathbf{a}_1 \times \mathbf{a}_2)$$

The following vector relation, found in many textbooks, is useful here:

$$\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B}(\mathbf{A} \cdot \mathbf{C}) - \mathbf{C}(\mathbf{A} \cdot \mathbf{B})$$

Compare the vectors that occur in the relation above to the numerator:

$$\mathbf{A} = \mathbf{a}_3 \times \mathbf{a}_1$$
$$\mathbf{B} = \mathbf{a}_1$$
$$\mathbf{C} = \mathbf{a}_2$$

After the substitution:

$$(\mathbf{a}_3 \times \mathbf{a}_1) \times (\mathbf{a}_1 \times \mathbf{a}_2) = \mathbf{a}_1[(\mathbf{a}_3 \times \mathbf{a}_1) \cdot \mathbf{a}_2] - \mathbf{a}_2[(\mathbf{a}_3 \times \mathbf{a}_1) \cdot \mathbf{a}_1]$$
$$= \mathbf{a}_1[\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)] + \mathbf{a}_2[(\mathbf{a}_1 \times \mathbf{a}_1) \cdot \mathbf{a}_3]$$

To arrive at this first term in the second expression of the right-hand side:

$$\mathbf{A} \cdot (\mathbf{B} \times \mathbf{C}) = (\mathbf{A} \times \mathbf{B}) \cdot \mathbf{C}$$

Note that the part of this term in brackets is now identical to the expression for the denominator. Also, the second term is equal to zero since we have a vector in a cross-product with itself. The result for $\mathbf{b}_2 \times \mathbf{b}_3$ is now:

$$\mathbf{b}_2 \times \mathbf{b}_3 = 4\pi^2 \mathbf{a}_1$$

Using the same method for the other relevant cross-products:

$$\mathbf{b}_3 \times \mathbf{b}_1 = 4\pi^2 \mathbf{a}_2$$
$$\mathbf{b}_1 \times \mathbf{b}_2 = 4\pi^2 \mathbf{a}_3$$

The denominators of (1), (2), and (3), may be solved using the cross-products above:

$$\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3) = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \cdot 4\pi^2 \mathbf{a}_1$$
$$= 8\pi^3$$

By substituting the results into the right-hand side of (1), we see that the equation holds true, and similarly for (2) and (3).

20. Figure 8.15(b) shows a member of the lattice plane with Miller indices (110). The plane perpendicular to the reciprocal lattice vector is:

$$\mathbf{g} = \mathbf{b}_1 + \mathbf{b}_2$$

Eq. (8.33) gives the distance between planes:

$$d = \frac{2\pi}{|\mathbf{g}|}$$

Using the primitive reciprocal vectors from Example 8.1,the magnitude of g is:

$$\mathbf{g} = \frac{2\pi}{a}\hat{i} + \frac{2\pi}{a}\hat{j} \Rightarrow |\mathbf{g}| = \sqrt{2}\frac{2\pi}{a}$$

Hence, the distance between planes is:

$$d = \frac{a}{\sqrt{2}} = \frac{\sqrt{2}a}{2}$$

21. Similarly to the previous problem, the plane perpendicular to the reciprocal lattice vector is:

$$\mathbf{g} = 2\mathbf{b}_1 + \mathbf{b}_2$$

Eq. (8.33) gives the distance between planes:

$$d = \frac{2\pi}{|\mathbf{g}|}$$

Using the primitive reciprocal vectors from Example 8.1,the magnitude of g is:

$$\mathbf{g} = \frac{4\pi}{a}\hat{\imath} + \frac{2\pi}{a}\hat{\jmath} \Rightarrow |\mathbf{g}| = \sqrt{5}\frac{2\pi}{a}$$

Hence, the distance between planes is:

$$d = \frac{a}{\sqrt{5}}$$

22.a) First let $g = g'$. Then $n(2\pi)/a = m(2\pi)/a$ or $n = m$ and:

$$\int_0^a e^{-ig'x}e^{igx}\ dx = \int_0^a e^{(n-m)2\pi x/a}\ dx = \int_0^a dx = a$$

On the other hand, if $g \neq g'$, let $j = n - m$ (an integer) and:

$$\int_0^a e^{-ig'x}e^{igx}\ dx = \int_0^a e^{j(2\pi i)x/a}\ dx$$

The integrand may be written using Euler's formula:

$$\int_0^a \cos(j2\pi x/a) + i\ \sin(j2\pi x/a))dx$$

and both functions (sin and cos) are integrated over a full cycle, so

$$\int_0^a e^{-ig'x}e^{igx}\ dx = 0$$

b) Using Eq. 8.14:

$$f(x) = \sum_g F_g e^{igx}$$

Multiply by $e^{-ig'x}$:

$$e^{-ig'x}f(x) = \sum_g F_g e^{-ig'x} e^{igx}$$

Integrating this:

$$\int_0^a e^{-ig'x} f(x)\ dx = \sum_g F_g \int_0^a e^{-ig'x} e^{igx}\ dx = \sum_g F_g a \delta_{gg'} = aF_{g'}$$

23. First, project the vector $\mathbf{l}$ onto $\mathbf{g}$:

$$d = \mathbf{l} \cdot \frac{\mathbf{g}}{|\mathbf{g}|} = \frac{2\pi N}{|\mathbf{g}|}$$

and similarly for $\mathbf{l}'$:

$$d' = \mathbf{l}' \cdot \frac{\mathbf{g}}{|\mathbf{g}|} = \frac{2\pi(N+1)}{|\mathbf{g}|}$$

The distance between the planes containing these points is:

$$d' - d = \frac{1}{|\mathbf{g}|}(2\pi(N+1) - 2\pi N) = \frac{2\pi}{|\mathbf{g}|}$$

24. Starting from Eq. (8.45):

$$\psi_k(x) = A_k e^{ikx}$$

where from Eq. (8.44), $k = 2\pi n/(Na)$ for integer n. Setting $A_k^2 = 1/L$:

$$\begin{aligned} \psi^*_{k'}(x)\psi_k(x) =& \frac{1}{L} e^{i(k-k')x} \\ =& \frac{1}{L}\left(\cos 2\pi(n-n')\frac{x}{Na} + i\ \sin 2\pi(n-n')\frac{x}{Na}\right) \end{aligned}$$

where the crystal length is $L = Na$. Integrating:

$$\frac{1}{L}\int_0^L \left(\cos 2\pi(n-n')\frac{x}{Na} + i\ \sin 2\pi(n-n')\frac{x}{Na}\right)\ dx = 0$$

since each function (sin and cos) is integrated over a full cycle. Hence, when $n \neq n'$, the orthogonality condition of Eq. (8.48) is satisfied.

25.a) Block's Theorem states:

$$\psi_k(\mathbf{r} + \mathbf{l}) = e^{i\mathbf{k}\cdot\mathbf{l}}\psi_k(\mathbf{r})$$

Let $\mathbf{l} = N_1\mathbf{a}_1$, giving:

$$\psi_k(\mathbf{r} + N_1\mathbf{a}_1) = e^{i\mathbf{k}\cdot N_1\mathbf{a}_1}\psi_k(\mathbf{r})$$

Using the Born-von Karman boundary condition:

$$\psi_k(\mathbf{r}) = e^{i\mathbf{k}\cdot N_1\mathbf{a}_1}\psi_k(\mathbf{r})$$

resulting in $e^{i\mathbf{k}\cdot N_1\mathbf{a}_1} = 1$, and similarly for $N_2\mathbf{a}_2$ and $N_3\mathbf{a}_3$.

b) For $\mathbf{k}$ given by Eq. (8.50):

$$\mathbf{k} = \frac{n_1}{N_1}\mathbf{b}_1 + \frac{n_2}{N_2}\mathbf{b}_2 + \frac{n_3}{N_3}\mathbf{b}_3$$

Then the dot product gives:

$$\mathbf{k}\cdot(N_1\mathbf{a}_1) = \left(\frac{n_1}{N_1}\right) N_1\mathbf{b}_1\cdot\mathbf{a}_1$$

and comparing this with Eqs. (8.34) and (8.35) gives:

$$\mathbf{k}\cdot(N_1\mathbf{a}_1) = n_1(2\pi)$$

Hence, we get $e^{2\pi i} = 1$, which is just Euler's identity, so this choice of $\mathbf{k}$ satisfies the conditions given in part (a).

26. Starting with Eqs. (8.51):

$$\psi_k(\mathbf{r}) = \frac{1}{V^{1/2}}e^{i\mathbf{k}\cdot\mathbf{r}}$$

gives:

$$\psi_{k'}(\mathbf{r}) = \frac{1}{V^{1/2}}e^{i\mathbf{k}'\cdot\mathbf{r}} \quad \text{and} \quad \psi_k^*(\mathbf{r}) = \frac{1}{V^{1/2}}e^{-i\mathbf{k}\cdot\mathbf{r}}$$

Then from Eq. (8.54):

$$V(\mathbf{r}) = \sum_g V_g e^{i\mathbf{g}\cdot\mathbf{r}}$$

and substituting these into the integral:

$$I^*_{k',\,k} = \sum_g \frac{V_g}{V}\int e^{i(\mathbf{g}+\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}\, dV$$

Separating the exponential terms:

$$I^*_{k',\,k} = \sum_g \frac{V_g}{V}\int e^{i(\mathbf{g}+\mathbf{k}')\cdot\mathbf{r}}e^{-i\mathbf{k}\cdot\mathbf{r}}\, dV$$

This can be rewritten as:

$$\sum_g \frac{V_g}{V} \int \psi^*_{\mathbf{k}}(\mathbf{r}) \psi_{(\mathbf{k}'+\mathbf{g})}(\mathbf{r})\ dV$$

and using the orthogonality condition of Eq. (8.58):

$$\mathbf{k} = \mathbf{k}' + \mathbf{g}$$

and the result of Problem 24 gives the desired orthogonality properties.

27. The band gap ΔE between the occupied and unoccupied states is at energies that correspond to infrared light. Since electrons must jump over the band gap to get into the conduction band, infrared light does not have enough energy to do this. Hence, infrared light will not create a quantum excitation and has a low probability of being absorbed by a semiconductor. On the other hand, visible light has enough energy to excite and electron into the conduction band. So photons of visible light frequencies will cause quantum excitations in a semiconductor and are readily absorbed, thereby the semiconductor is opaque to visible light.