CHAPTER 3
STRUCTURES OF METALS AND CERAMICS
PROBLEM SOLUTIONS

Point Coordinates
3.22 List the point coordinates of both the sodium and chlorine ions for a unit cell of the sodium chloride crystal structure (Figure 3.5).

Solution
Here we are asked to list point coordinates for both sodium and chlorine ions for a unit cell of the sodium chloride crystal structure, which is shown in Figure 3.5.

In Figure 3.5, the chlorine ions are situated at all corners and face-centered positions. Therefore, point coordinates for these ions are the same as for FCC, as presented in the previous problem—that is, 000, 100, 110, 010, 001, 101, 111, 011, \( \frac{1}{2} 0 0 \), \( \frac{1}{2} 1 0 \), \( \frac{1}{2} 1 1 \), \( \frac{1}{2} 0 \frac{1}{2} \), \( \frac{1}{2} \frac{1}{2} \), \( \frac{1}{2} 0 \frac{1}{2} \), and \( \frac{1}{2} \frac{1}{2} \).

Furthermore, the sodium ions are situated at the centers of all unit cell edges, and, in addition, at the unit cell center. For the bottom face of the unit cell, the point coordinates are as follows: \( \frac{1}{2} 0 0 \), \( \frac{1}{2} \frac{1}{2} \), \( \frac{1}{2} \frac{1}{2} \), \( \frac{1}{2} 0 \), and \( 0 \frac{1}{2} \). While, for the horizontal plane that passes through the center of the unit cell (which includes the ion at the unit cell center), the coordinates are \( 00 \frac{1}{2} \), \( 0 \frac{1}{2} \), \( \frac{1}{2} \frac{1}{2} \), \( \frac{1}{2} 0 \), \( \frac{1}{2} 1 \), and \( \frac{1}{2} \frac{1}{2} \). And for the four ions on the top face \( \frac{1}{2} 0 1 \), \( \frac{1}{2} \frac{1}{2} \), \( \frac{1}{2} \frac{1}{2} \), and \( 0 \frac{1}{2} \).

3.27 Within a cubic unit cell, sketch the following directions:

(a) \([102]\),
(b) \([313]\),
(c) \([212]\),
(d) \([301]\).

Solution
The directions asked for are indicated in the cubic unit cell shown below.

3.31 Determine the indices for the two directions shown in the following hexagonal unit cell:
Solution

For direction A, projections on the $a_1$, $a_2$, and $z$ axes are $a$, $0a$, and $c/2$, or, in terms of $a$ and $c$ the projections are 1, 0, and 1/2, which when multiplied by the factor 2 become the smallest set of integers: 2, 0, and 1. This means that

$$u' = 2$$
$$v' = 0$$
$$w' = 1$$

Now, from Equations 3.7, the $u$, $v$, $t$, and $w$ indices become

$$u = \frac{1}{3}(2u' - v') = \frac{1}{3}(2(2) - 0) = \frac{4}{3}$$
$$v = \frac{1}{3}(2v' - u') = \frac{1}{3}[2(0) - (2)] = \frac{-2}{3}$$
$$t = -(u+v) = -\left(\frac{4}{3} + \frac{-2}{3}\right) = \frac{-2}{3}$$
$$w = w' = 1$$

Now, in order to get the lowest set of integers, it is necessary to multiply all indices by the factor 3, with the result that the direction A is a $[4\bar{2}23]$ direction.

For direction B, projections on the $a_1$, $a_2$, and $z$ axes are $-a$, $0a$, and $0c$, or, in terms of $a$ and $c$ the projections are $-1$, 0, and 0. This means that

$$u' = -1$$
$$v' = 0$$
$$w' = 0$$

Now, from Equations 3.7, the $u$, $v$, $t$, and $w$ indices become

$$u = \frac{1}{3}(2u' - v') = \frac{1}{3}(2(-1) - 0) = \frac{-2}{3}$$
$$v = \frac{1}{3}(2v' - u') = \frac{1}{3}[2(0) - (-1)] = \frac{1}{3}$$
$$t = -(u+v) = -\left(\frac{-2}{3} + \frac{1}{3}\right) = \frac{1}{3}$$
$$w = w' = 0$$

Now, in order to get the lowest set of integers, it is necessary to multiply all indices by the factor 3, with the result that the direction B is a $[\bar{2}110]$ direction.

3.35 Sketch within a cubic unit cell the following planes:

(a) $(012)$,  
(b) $(3\bar{1}3)$,
(c) $(10\bar{1})$,  
(d) $(2\bar{1}1)$. 

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3.37 Determine the Miller indices for the planes shown in the following unit cell:

Solution

For plane A since the plane passes through the origin of the coordinate system as shown, we will move the origin of the coordinate system one unit cell distance vertically along the z axis; thus, this is a (211) plane, as summarized below.

For plane B, since the plane passes through the origin of the coordinate system as shown, we will move the origin one unit cell distance vertically along the z axis; this is a (021) plane, as summarized below.
3.44  (a) Derive planar density expressions for BCC (100) and (110) planes in terms of the atomic radius $R$.

(b) Compute and compare planar density values for these same two planes for molybdenum.

Solution
(a) A BCC unit cell within which is drawn a (100) plane is shown below.

For this (100) plane there is one atom at each of the four cube corners, each of which is shared with four adjacent unit cells. Thus, there is the equivalence of 1 atom associated with this BCC (100) plane. The planar section represented in the above figure is a square, wherein the side lengths are equal to the unit cell edge length, $\frac{4R}{\sqrt{3}}$ (Equation 3.3); and, thus, the area of this square is just $\left(\frac{4R}{\sqrt{3}}\right)^2 = \frac{16R^2}{3}$. Hence, the planar density for this (100) plane is just

$$PD_{100} = \frac{\text{number of atoms centered on (100) plane}}{\text{area of (100) plane}} = \frac{1 \text{ atom}}{16 \frac{R^2}{3}} = \frac{3}{16 \frac{R^2}{3}}$$

A BCC unit cell within which is drawn a (110) plane is shown below.

For this (110) plane there is one atom at each of the four cube corners through which it passes, each of which is shared with four adjacent unit cells, while the center atom lies entirely within the unit cell. Thus,
there is the equivalence of 2 atoms associated with this BCC (110) plane. The planar section represented in the above figure is a rectangle, as noted in the figure below.

From this figure, the area of the rectangle is the product of $x$ and $y$. The length $x$ is just the unit cell edge length, which for BCC (Equation 3.3) is $\frac{4R}{\sqrt{3}}$. Now, the diagonal length $z$ is equal to $4R$. For the triangle bounded by the lengths $x$, $y$, and $z$

$y = \sqrt{z^2 - x^2}$

Or

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

Thus, in terms of $R$, the area of this (110) plane is just

$\text{Area (110)} = xy = \left(\frac{4R}{\sqrt{3}}\right)\left(\frac{4R\sqrt{2}}{\sqrt{3}}\right) = \frac{16R^2\sqrt{2}}{3}$

And, finally, the planar density for this (110) plane is just

$PD_{110} = \frac{\text{number of atoms centered on (110) plane}}{\text{area of (110) plane}}$

$\quad = \frac{2 \text{ atoms}}{\frac{16R^2\sqrt{2}}{3}} = \frac{3}{8R^2\sqrt{2}}$

(b) From the table inside the front cover, the atomic radius for molybdenum is 0.136 nm. Therefore, the planar density for the (100) plane is

$PD_{100}(\text{Mo}) = \frac{3}{16R^2} = \frac{3}{16(0.136 \text{ nm})^2} = 10.14 \text{ nm}^{-2} = 1.014 \times 10^{19} \text{ m}^{-2}$

While for the (110) plane

$PD_{110}(\text{Mo}) = \frac{3}{8R^2\sqrt{2}} = \frac{3}{8(0.136 \text{ nm})^2\sqrt{2}} = 14.34 \text{ nm}^{-2} = 1.434 \times 10^{19} \text{ m}^{-2}$