CHAPTER 3

FUNDAMENTALS OF CRYSTALLOGRAPHY

PROBLEM SOLUTIONS

Fundamental Concepts

3.1 What is the difference between atomic structure and crystal structure?

Solution

Atomic structure relates to the number of protons and neutrons in the nucleus of an atom, as well as the number and probability distributions of the constituent electrons. On the other hand, crystal structure pertains to the arrangement of atoms in the crystalline solid material.
Crystal Systems

3.2 The accompanying figure shows a unit cell for a hypothetical metal.
(a) To which crystal system does this unit cell belong?
(b) What would this crystal structure be called?
(c) Calculate the density of the material, given that its atomic weight is 145 g/mol.

Solution

(a) The unit cell shown in the problem statement belongs to the tetragonal crystal system since
\( a = b = 0.30 \text{ nm}, \ c = 0.40 \text{ nm}, \ \text{and} \ \alpha = \beta = \gamma = 90^\circ. \)
(b) The crystal structure would be called \textit{body-centered tetragonal}.
(c) As with BCC, \( n = 2 \) atoms/unit cell. Also, for this unit cell

\[
V_C = (3.0 \times 10^{-8} \text{ cm})^2 (4.0 \times 10^{-8} \text{ cm})
\]

\[
= 3.60 \times 10^{-23} \text{ cm}^3/\text{unit cell}
\]

Thus, using Equation 4.8, the density is equal to

\[
\frac{nA}{V_C N_A} = \frac{(2 \text{ atoms/unit cell})(145 \text{ g/mol})}{(3.60 \times 10^{-23} \text{ cm}^3/\text{unit cell})(6.022 \times 10^{23} \text{ atoms/mol})}
\]

\[
= 13.38 \text{ g/cm}^3
\]
3.3 Sketch a unit cell for the body-centered orthorhombic crystal structure.

Solution

A unit cell for the body-centered orthorhombic crystal structure is presented below.
Point Coordinates

3.4 List the point coordinates for all atoms that are associated with the FCC unit cell (Figure 3.1).

Solution

From Figure 3.1b, the atom located at the origin of the unit cell has the coordinates 000. Coordinates for other atoms in the bottom face are 100, 110, 010, and $1\frac{1}{2}0$. (The $z$ coordinate for all these points is zero.)

For the top unit cell face, the coordinates are 001, 101, 111, 011, and $1\frac{1}{2}1$.

Coordinates for those atoms that are positioned at the centers of both side faces, and centers of both front and back faces need to be specified. For the front and back-center face atoms, the coordinates are $1\frac{1}{2}2$ and $0\frac{1}{2}2$, respectively. While for the left and right side center-face atoms, the respective coordinates are $1\frac{1}{2}0$ and $1\frac{1}{2}1$.
3.5 List the point coordinates of the titanium, barium, and oxygen ions for a unit cell of the perovskite crystal structure (Figure 4.9).

Solution

In Figure 4.9, the barium ions are situated at all corner positions. The point coordinates for these ions are as follows: 000, 100, 110, 010, 001, 101, 111, and 011.

The oxygen ions are located at all face-centered positions; therefore, their coordinates are
\[
\frac{1}{2} \frac{1}{2} 0, \frac{1}{2} \frac{1}{2} 1, \frac{1}{2} \frac{1}{2} 2, 0 \frac{1}{2} \frac{1}{2}, \frac{1}{2} 0 \frac{1}{2}, \text{ and } \frac{1}{2} \frac{1}{2} \frac{1}{2}.
\]

And, finally, the titanium ion resides at the center of the cubic unit cell, with coordinates
\[
\frac{1}{2} \frac{1}{2} \frac{1}{2}.
\]
3.6 List the point coordinates of all atoms that are associated with the diamond cubic unit cell (Figure 4.17).

Solution

First of all, one set of carbon atoms occupy all corner positions of the cubic unit cell; the coordinates of these atoms are as follows: 000, 100, 110, 010, 001, 101, 111, and 011.

Another set of atoms reside on all of the face-centered positions, with the following coordinates: \( \frac{1}{2}, \frac{1}{2}, 0 \), \( \frac{1}{2}, \frac{1}{2}, 1 \), \( \frac{1}{2}, 0, \frac{1}{2} \), \( \frac{1}{2}, 1, \frac{1}{2} \), \( 0, \frac{1}{2}, \frac{1}{2} \), \( \frac{1}{2}, 0, \frac{1}{2} \), and \( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \).

The third set of carbon atoms are positioned within the interior of the unit cell. Using an x-y-z coordinate system oriented as in Figure 3.2, the coordinates of the atom that lies toward the lower-left-front of the unit cell has the coordinates \( \frac{3}{4}, \frac{1}{4}, \frac{1}{4} \), whereas the atom situated toward the lower-right-back of the unit cell has coordinates of \( \frac{1}{4}, \frac{3}{4}, \frac{3}{4} \). Also, the carbon atom that resides toward the upper-left-back of the unit cell has the coordinates \( \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \). And, the coordinates of the final atom, located toward the upper-right-front of the unit cell, are \( \frac{3}{4}, \frac{3}{4}, \frac{3}{4} \).
3.7 Sketch a tetragonal unit cell, and within that cell indicate locations of the $\frac{1}{2} \frac{1}{2}$ and $\frac{1}{4} \frac{3}{4}$ point coordinates.

Solution

A tetragonal unit in which are shown the $\frac{1}{2} \frac{1}{2}$ and $\frac{1}{4} \frac{3}{4}$ point coordinates is presented below.

![Diagram of a tetragonal unit cell with indicated point coordinates]
3.8 Using the Molecule Definition Utility found in both “Metallic Crystal Structures and Crystallography” and “Ceramic Crystal Structures” modules of VMSE, available in WileyPlus, generate a three-dimensional unit cell for the intermetallic compound AuCu₃, given the following: (1) the unit cell is cubic with an edge length of 0.374 nm, (2) gold atoms are situated at all cube corners, and (3) copper atoms are positioned at the centers of all unit cell faces.

Solution

First of all, open the “Molecular Definition Utility”; it may be found in either of “Metallic Crystal Structures and Crystallography” or “Ceramic Crystal Structures” modules.

In the “Step 1” window, it is necessary to define the atom types, colors for the spheres (atoms), and specify atom sizes. Let us enter “Au” as the name for the gold atoms (since Au is the symbol for gold), and “Cu” as the name for the copper atoms. Next it is necessary to choose a color for each atom type from the selections that appear in the pull-down menu—for example, “Yellow” for Au and “Red” for Cu. In the “Atom Size” window, it is necessary to enter an atom/ion size. In the instructions for this step, it is suggested that the atom/ion diameter in nanometers be used. From the table found inside the front cover of the textbook, the atomic radii for gold and copper are 0.144 nm and 0.128 nm, respectively, and, therefore, their ionic diameters are twice these values (i.e., 0.288 nm and 0.256 nm); therefore, we enter the values “0.288” and “0.256” for the two atom types. Now click on the “Register” button, followed by clicking on the “Go to Step 2” button.

In the “Step 2” window we specify positions for all of the atoms within the unit cell; their point coordinates are specified in the problem statement. Let’s begin with gold. Click on the yellow sphere that is located to the right of the “Molecule Definition Utility” box. Again, Au atoms are situated at all eight corners of the cubic unit cell. One Au will be positioned at the origin of the coordinate system—i.e., its point coordinates are 000, and, therefore, we enter a “0” (zero) in each of the “x”, “y”, and “z” atom position boxes. Next we click on the “Register Atom Position” button. Now we enter the coordinates of another gold atom; let us arbitrarily select the one that resides at the corner of the unit cell that is one unit-cell length along the x-axis (i.e., at the 100 point coordinate). Inasmuch as it is located a distance of a units along the x-axis the value of “0.374” is entered in the “x” atom position box (since this is the value of a given in the problem statement); zeros are entered in each of the “y” and “z” position boxes. We repeat this procedure for the remaining six Au atoms.

After this step has been completed, it is necessary to specify positions for the copper atoms, which are located at all six face-centered sites. To begin, we click on the red sphere that is located next to the “Molecule Definition Utility” box. The point coordinates for some of the Cu atoms are fractional ones; in these instances, the a unit cell length (i.e., 0.374) is multiplied by the fraction. For example, one Cu atom is located 1 1/2 1/2 coordinate. Therefore, the x, y, and z atoms positions are (1)(0.374) = 0.374, 1/2(0.374) = 0.187, and 1/2(0.374) = 0.187, respectively.
For the gold atoms, the x, y, and z atom position entries for all 8 sets of point coordinates are as follows:

0, 0, 0
0.374, 0, 0
0, 0.374, 0
0, 0, 0.374
0, 0.374, 0.374
0.374, 0, 0.374
0.374, 0.374, 0
0.374, 0.374, 0.374

Now, for the copper atoms, the x, y, and z atom position entries for all 6 sets of point coordinates are as follows:

0.187, 0.187, 0
0.187, 0, 0.187
0, 0.187, 0.187
0.374, 0.187, 0.187
0.187, 0.374, 0.187
0.187, 0.187, 0.374

In Step 3, we may specify which atoms are to be represented as being bonded to one another, and which type of bond(s) to use (single solid, single dashed, double, and triple are possibilities), or we may elect to not represent any bonds at all (in which case we are finished). If it is decided to show bonds, probably the best thing to do is to represent unit cell edges as bonds. This image may be rotated by using mouse click-and-drag.

Your image should appear as the following screen shot. Here the gold atoms appear lighter than the copper atoms.
[Note: Unfortunately, with this version of the Molecular Definition Utility, it is not possible to save either the data or the image that you have generated. You may use screen capture (or screen shot) software to record and store your image.]
Crystallographic Directions

3.9 Draw an orthorhombic unit cell, and within that cell a \([12\overline{1}]\) direction.

**Solution**

This problem calls for us to draw a \([12\overline{1}]\) direction within an orthorhombic unit cell \((a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ)\). Such a unit cell with its origin positioned at point O is shown below. We first move along the +x-axis \(a\) units (from point O to point A), then parallel to the +y-axis \(2b\) units (from point A to point B). Finally, we proceed parallel to the z-axis \(-c\) units (from point B to point C). The \([12\overline{1}]\) direction is the vector from the origin (point O) to point C as shown.
3.10 Sketch a monoclinic unit cell, and within that cell a [011] direction.

Solution

This problem asks that a [011] direction be drawn within a monoclinic unit cell ($a \neq b \neq c$, and $\alpha = \beta = 90^\circ \neq \gamma$). One such unit cell with its origin at point $O$ is sketched below. For this direction, there is no projection along the $x$-axis since the first index is zero; thus, the direction lies in the $y$-$z$ plane. We next move from the origin along the minus $y$-axis $b$ units (from point $O$ to point $R$). Since the final index is a one, move from point $R$ parallel to the $z$-axis, $c$ units (to point $P$). Thus, the [011] direction corresponds to the vector passing from the origin (point $O$) to point $P$, as indicated in the figure.
3.11 What are the indices for the directions indicated by the two vectors in the following sketch?

![Diagram of two vectors]

**Solution**

This is a [012] direction as indicated in the summary below.

<table>
<thead>
<tr>
<th></th>
<th>( \hat{x} )</th>
<th>( \hat{y} )</th>
<th>( \hat{z} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Head</td>
<td>0a</td>
<td>( b/2 )</td>
<td>( c )</td>
</tr>
<tr>
<td>coordinates (( x_2 ), ( y_2 ), ( z_2 ))</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tail</td>
<td>0a</td>
<td>0b</td>
<td>0c</td>
</tr>
<tr>
<td>coordinates (( x_1 ), ( y_1 ), ( z_1 ))</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Coordinate differences</td>
<td>0a</td>
<td>( b/2 )</td>
<td>( c )</td>
</tr>
<tr>
<td>Calculated values of ( u ), ( v ), and ( w )</td>
<td>( u = 0 )</td>
<td>( v = 1 )</td>
<td>( w = 2 )</td>
</tr>
<tr>
<td>Enclosure</td>
<td></td>
<td></td>
<td>[012]</td>
</tr>
</tbody>
</table>

Direction 2 is [11\( \frac{2}{2} \)] as summarized below.

<table>
<thead>
<tr>
<th></th>
<th>( \hat{x} )</th>
<th>( \hat{y} )</th>
<th>( \hat{z} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Head</td>
<td>( a/2 )</td>
<td>( b/2 )</td>
<td>( -c )</td>
</tr>
<tr>
<td>coordinates (( x_2 ), ( y_2 ), ( z_2 ))</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tail</td>
<td>0a</td>
<td>0b</td>
<td>0c</td>
</tr>
<tr>
<td>coordinates (( x_1 ), ( y_1 ), ( z_1 ))</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Coordinate differences</td>
<td>( a/2 )</td>
<td>( b/2 )</td>
<td>( -c )</td>
</tr>
<tr>
<td>Calculated values of ( u ), ( v ), and ( w )</td>
<td>( u = 1 )</td>
<td>( v = 1 )</td>
<td>( w = -2 )</td>
</tr>
<tr>
<td>Enclosure</td>
<td></td>
<td></td>
<td>[11( \frac{2}{2} )]</td>
</tr>
</tbody>
</table>
3.12 Within a cubic unit cell, sketch the following directions:

(a) $[\overline{1}10]$, (e) $[\overline{1}1]$, 
(b) $[\overline{1}21]$, (f) $[\overline{1}22]$, 
(c) $[0\overline{1}2]$, (g) $[1\overline{2}3]$, 
(d) $[1\overline{3}3]$, (h) $[\overline{1}03]$. 

**Solution**

The directions asked for are indicated in the cubic unit cells shown below.
3.13 Determine the indices for the directions shown in the following cubic unit cell:

**Solution**

Direction A is a \([0\bar{1}1]\) direction. To solve this problem, we first take note of the vector tail and head coordinates, then take the point coordinate differences. We then use Equation 3.2 selecting a value of \(n\) that will produce integer values of \(u\), \(v\), and \(w\). In this case select \(n = 1\) as there are no fractions in the differences. Finally, the values of \(u\), \(v\), and \(w\) are enclosed in brackets to give the direction designation. This is summarized as follows:

<table>
<thead>
<tr>
<th>(\bar{x})</th>
<th>(\bar{y})</th>
<th>(\bar{z})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Head coordinates ((x_2, y_2, z_2))</td>
<td>0a</td>
<td>0b</td>
</tr>
<tr>
<td>Tail coordinates ((x_1, y_1, z_1))</td>
<td>0a</td>
<td>(b)</td>
</tr>
<tr>
<td>Coordinate differences</td>
<td>0a</td>
<td>(-b)</td>
</tr>
<tr>
<td>Calculated values of (u), (v), and (w)</td>
<td>(u = 0)</td>
<td>(v = -1)</td>
</tr>
<tr>
<td>Enclosure</td>
<td>([0\bar{1}1])</td>
<td></td>
</tr>
</tbody>
</table>

Direction B is a \([\bar{2}10]\) direction as indicated in the summary below.

<table>
<thead>
<tr>
<th>(\bar{x})</th>
<th>(\bar{y})</th>
<th>(\bar{z})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Head coordinates ((x_2, y_2, z_2))</td>
<td>0a</td>
<td>(b)</td>
</tr>
<tr>
<td>Tail coordinates ((x_1, y_1, z_1))</td>
<td>(a)</td>
<td>(b/2)</td>
</tr>
<tr>
<td>Coordinate differences</td>
<td>(-a)</td>
<td>(b/2)</td>
</tr>
<tr>
<td>Calculated values of (u), (v), and (w)</td>
<td>(u = -2)</td>
<td>(v = 1)</td>
</tr>
<tr>
<td>Enclosure</td>
<td>([\bar{2}10])</td>
<td></td>
</tr>
</tbody>
</table>
Direction C is a [112] direction as indicated in the summary below.

<table>
<thead>
<tr>
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<th>(x)</th>
<th>(y)</th>
<th>(z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Head</td>
<td>(a)</td>
<td>(b)</td>
<td>(c)</td>
</tr>
<tr>
<td>Tail</td>
<td>(a/2)</td>
<td>(b/2)</td>
<td>(0c)</td>
</tr>
<tr>
<td>Differences</td>
<td>(a/2)</td>
<td>(b/2)</td>
<td>(c)</td>
</tr>
<tr>
<td>Calculated values of (u), (v), and (w)</td>
<td>(u = 1)</td>
<td>(v = 1)</td>
<td>(w = 2)</td>
</tr>
</tbody>
</table>

Enclosure:

Direction D is a [11\(\overline{2}\)] direction as indicated in the summary below.

<table>
<thead>
<tr>
<th></th>
<th>(x)</th>
<th>(y)</th>
<th>(z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Head</td>
<td>(a)</td>
<td>(b/2)</td>
<td>(0c)</td>
</tr>
<tr>
<td>Tail</td>
<td>(a/2)</td>
<td>(0b)</td>
<td>(c)</td>
</tr>
<tr>
<td>Differences</td>
<td>(a/2)</td>
<td>(b/2)</td>
<td>(-c)</td>
</tr>
<tr>
<td>Calculated values of (u), (v), and (w)</td>
<td>(u = 1)</td>
<td>(v = 1)</td>
<td>(w = -2)</td>
</tr>
</tbody>
</table>

Enclosure:

[11\(\overline{2}\)]
3.14 Determine the indices for the directions shown in the following cubic unit cell:

Solution

Direction A is a $[\bar{4}30]$ direction. To solve this problem, we first take note of the vector tail and head coordinates, then take the point coordinate differences. We then use Equation 3.2 selecting a value of $n$ that will produce integer values of $u$, $v$, and $w$. In this case select $n = 1$ as there are no fractions in the differences. Finally, the values of $u$, $v$, and $w$ are enclosed in brackets to give the direction designation. This is summarized as follows:

$$
\begin{array}{ccc}
\bar{x} & \bar{y} & \bar{z} \\
\text{Head coordinates (}x_2, y_2, z_2) & 0a & b/2 & c \\
\text{Tail coordinates (}x_1, y_1, z_1) & 2a/3 & 0b & c \\
\text{Coordinate differences} & -2a/3 & b/2 & 0c \\
\text{Calculated values of } u, v, \text{ and } w & u = -4 & v = 3 & w = 0 \\
\text{Enclosure} & [\bar{4}30] \\
\end{array}
$$

Direction B is a $[2\bar{3}2]$ direction as indicated in the summary below.

$$
\begin{array}{ccc}
\bar{x} & \bar{y} & \bar{z} \\
\text{Head coordinates (}x_2, y_2, z_2) & a & 0b & 2c/3 \\
\text{Tail coordinates (}x_1, y_1, z_1) & a/3 & b & 0c \\
\text{Coordinate differences} & 2a/3 & -b & 2c/3 \\
\text{Calculated values of } u, v, \text{ and } w & u = 2 & v = -3 & w = 2 \\
\text{Enclosure} & [2\bar{3}2] \\
\end{array}
$$
Direction C is a \([1\overline{3}3]\) direction as indicated in the summary below.

<table>
<thead>
<tr>
<th>(\xi)</th>
<th>(\eta)</th>
<th>(\zeta)</th>
</tr>
</thead>
<tbody>
<tr>
<td>((x_2, y_2, z_2))</td>
<td>(2a/3)</td>
<td>(0b)</td>
</tr>
<tr>
<td>((x_1, y_1, z_1))</td>
<td>(a/3)</td>
<td>(b)</td>
</tr>
<tr>
<td>Coordinate differences</td>
<td>(a/3)</td>
<td>(-b)</td>
</tr>
<tr>
<td>Calculated values of (u), (v), and (w)</td>
<td>(u = 1)</td>
<td>(v = -3)</td>
</tr>
<tr>
<td>Enclosure</td>
<td>([1\overline{3}3])</td>
<td></td>
</tr>
</tbody>
</table>

Direction D is a \([1\overline{3}6]\) direction as indicated in the summary below.

<table>
<thead>
<tr>
<th>(\xi)</th>
<th>(\eta)</th>
<th>(\zeta)</th>
</tr>
</thead>
<tbody>
<tr>
<td>((x_2, y_2, z_2))</td>
<td>(a/2)</td>
<td>(b/2)</td>
</tr>
<tr>
<td>((x_1, y_1, z_1))</td>
<td>(a/3)</td>
<td>(0b)</td>
</tr>
<tr>
<td>Coordinate differences</td>
<td>(a/6)</td>
<td>(b/2)</td>
</tr>
<tr>
<td>Calculated values of (u), (v), and (w)</td>
<td>(u = 1)</td>
<td>(v = 3)</td>
</tr>
<tr>
<td>Enclosure</td>
<td>([1\overline{3}6])</td>
<td></td>
</tr>
</tbody>
</table>
3.15 For tetragonal crystals, cite the indices of directions that are equivalent to each of the following directions:

(a) [001]
(b) [110]
(c) [010]

Solution

For tetragonal crystals $a = b \neq c$ and $\alpha = \beta = \gamma = 90^\circ$; therefore, projections along the $x$ and $y$ axes are equivalent, which are not equivalent to projections along the $z$ axis.

(a) Therefore, for the [001] direction, there is only one equivalent direction: [001].
(b) For the [110] direction, equivalent directions are as follows: [110], [110], and [110]
(b) Also, for the [010] direction, equivalent directions are the following: [010], [010], and [010].
3.16 Convert the [100] and [111] directions into the four-index Miller–Bravais scheme for hexagonal unit cells.

Solution

For [100]

\[ U = 1, \]
\[ V = 0, \]
\[ W = 0 \]

From Equations 3.6

\[ u = \frac{1}{3}(2U \quad V) = \frac{1}{3}[(2)(1) \quad 0] = \frac{2}{3} \]

\[ v = \frac{1}{3}(2V \quad U) = \frac{1}{3}[(2)(0) \quad 1] = \frac{1}{3} \]

\[ t = (u + v) = \frac{2}{3} + \frac{1}{3} = \frac{1}{3} \]

\[ w = W = 0 \]

It is necessary to multiply these numbers by 3 in order to reduce them to the lowest set of integers. Thus, the direction is represented as \([uvw] = [2\overline{1}0]\).

For [111], \(U = 1, V = 1, \) and \(W = 1\); therefore,

\[ u = \frac{1}{3}[(2)(1) \quad 1] = \frac{1}{3} \]

\[ v = \frac{1}{3}[(2)(1) \quad 1] = \frac{1}{3} \]

\[ t = \frac{1}{3} + \frac{1}{3} = \frac{2}{3} \]

\[ w = 1 \]

If we again multiply these numbers by 3, then \(u = 1, v = 1, t = -2, \) and \(w = 3\). Thus, the direction is represented as \([uvw] = [1\overline{1}23]\).
3.17 Determine indices for the directions shown in the following hexagonal unit cells:

**Solution**

(a) For this direction, head coordinates are \(a, a/2, \text{ and } c/2\) and tail coordinates are \(0a, 0a, \text{ and } 0c\) giving the calculated differences as \(a, a/2, \text{ and } c/2\). Using the factor \(n = 2\) in Equation 3.2 produces the smallest set of integers: 2, 1, and 1. This means that

\[
U = 2 \\
V = 1 \\
W = 1
\]

Now, from Equations 3.3, the \(u, v, t, \text{ and } w\) indices become

\[
u = \frac{1}{3}(2V - U) = \frac{1}{3}(2) - (2) = 0
\]

\[
u = \frac{1}{3}(2V - U) = \frac{1}{3}(2) - (2) = 0
\]

\[
u = \frac{1}{3}(2V - U) = \frac{1}{3}(2) - (2) = 0
\]

\[
u = \frac{1}{3}(2V - U) = \frac{1}{3}(2) - (2) = 0
\]

\[
u = \frac{1}{3}(2V - U) = \frac{1}{3}(2) - (2) = 0
\]

\[
u = \frac{1}{3}(2V - U) = \frac{1}{3}(2) - (2) = 0
\]

\[
u = \frac{1}{3}(2V - U) = \frac{1}{3}(2) - (2) = 0
\]

\[
u = \frac{1}{3}(2V - U) = \frac{1}{3}(2) - (2) = 0
\]

\[
u = \frac{1}{3}(2V - U) = \frac{1}{3}(2) - (2) = 0
\]

\[
u = \frac{1}{3}(2V - U) = \frac{1}{3}(2) - (2) = 0
\]

\[
u = \frac{1}{3}(2V - U) = \frac{1}{3}(2) - (2) = 0
\]

No reduction is necessary inasmuch as all of these indices are integers; therefore, this direction in the four-index scheme is \([10\overline{1}1]\)
(b) For this direction, head coordinates are $a/2$, $a$, and $0c$ and tail coordinates are $0a$, $0a$, and $0c$ giving the calculated differences as $a/2$, $a$, and $0c$. Using the factor $n = 2$ in Equation 3.2 produces the smallest set of integers: 1, 2, and 0. This means that

$$U = 1$$
$$V = 2$$
$$W = 0$$

Now, from Equations 3.3, the $u$, $v$, $t$, and $w$ indices become

$$u = \frac{1}{3}(2U - V) = \frac{1}{3}(2)(1) = 0$$

$$v = \frac{1}{3}(2V - U) = \frac{1}{3}(2)(2) = 1$$

$$t = (u+v) = (0+1) = 1$$

$$w = W = 0$$

No reduction is necessary inasmuch as all of these indices are integers; therefore, this direction in the four-index scheme is $[0110]$. 
(c) For this direction, head coordinates are \(-a, -a, \) and \(c/2\) and tail coordinates are \(0a, 0a, \) and \(0c\) giving the calculated differences as \(-a, a, \) and \(c/2\). Using the factor \(n = 2\) in Equation 3.2 produces the smallest set of integers: \(-2, -2, \) and \(1\). This means that

\[
U = -2 \\
V = -2 \\
W = 1
\]

Now, from Equations 3.3, the \(u, v, t, \) and \(w\) indices become

\[
u = \frac{1}{3}(2U - V) = \frac{1}{3}(2)(2) = \frac{2}{3}
\]

\[
v = \frac{1}{3}(2V - U) = \frac{1}{3}(2)(2) = \frac{2}{3}
\]

\[
t = (u + v) = \frac{2}{3} + \frac{2}{3} = \frac{4}{3}
\]

\[
w = W = 1
\]

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 this direction is a \([\frac{22}{3}43]\) direction.
(d) For this direction, head coordinates are \(0a, -a,\) and \(0c\) and tail coordinates are \(0a, 0a,\) and \(0c\) giving the calculated differences as \(0a, -a,\) and \(0c.\) Using the factor \(n = 1\) in Equation 3.2 produces the smallest set of integers: 0, -1, and 0. This means that

\[
U = 0 \\
V = -1 \\
W = 0
\]

Now, from Equations 3.3, the \(u, v, t,\) and \(w\) indices become

\[
u = \frac{1}{3}(2U - V) = \frac{1}{3}(2)(0) - (-1) = \frac{1}{3}
\]

\[
v = \frac{1}{3}(2V - U) = \frac{1}{3}(2)(-1) - 0 = -\frac{2}{3}
\]

\[
t = -(u+v) = \frac{1}{3} - \frac{2}{3} = \frac{1}{3}
\]

\[
w = W = 0
\]

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 this is a \([1210]\) direction.
3.18 Sketch the \([\overline{1} 23]\) and \([10\overline{1}0]\) directions in a hexagonal unit cell.

**Solution**

The first portion of this problem asks that we plot the \([\overline{1} 23]\) within a hexagonal unit cell. Below is shown this direction plotted within a hexagonal unit cell having a reduced-scale coordinate scheme.

For this direction, projections on the \(a_1\), \(a_2\), \(a_3\), and \(c\) axes are respectively, \(-1\), \(-1\), 2, and 3, respectively. In plotting this direction, we begin at the origin of the coordinate system, point \(o\). From here we proceed 1 unit distance along the \(-a_1\) axis (to point \(p\)), from here 1 unit distance parallel to \(-a_2\) axis (to point \(q\)), then 2 unit distances parallel (or along) the \(a_3\) axis (to point \(r\)), and finally, 3 unit distances parallel to the \(z\) axis (to point \(s\)). Thus, the \([\overline{1} 23]\) direction is that vector that extends from point \(o\) to point \(s\) as shown.

Now we are asked to plot the \([10\overline{1}0]\) within a hexagonal unit cell. In the figure below is plotted this direction within a hexagonal unit cell having a reduced-scale coordinate scheme.
For this direction, projections on the $a_1$, $a_2$, $a_3$, and $c$ axes are respectively, 1, 0, −1, and 0, respectively. In plotting this direction, we begin at the origin of the coordinate system, point $o$. From here we proceed 1 unit distance along the $a_1$ axis (to point $p$). Since there is no projection on the $a_2$ axis it is not necessary to move parallel to this axis. Therefore, from point $p$ we proceed 1 unit distance parallel to $−a_3$ axis (to point $q$). And, finally, inasmuch as there is no projection along the $z$ axis, it is not necessary to move parallel to this axis. Thus, the $[10\bar{1}0]$ direction is that vector that extends from point $o$ to point $q$ as shown.
3.19 Using Equations 3.3a, 3.3b, 3.3c, and 3.3d, derive expressions for each of the three primed indices set (U', V, and W) in terms of the four unprimed indices (u, v, t, and w).

**Solution**

It is first necessary to do an expansion of Equation 3.3a as

\[
   u = \frac{1}{3}(2U - V) = \frac{2U}{3} - \frac{V}{3}
\]

And solving this expression for V yields

\[
   V = 2U - 3u
\]

Now, substitution of this expression into Equation 3.3b gives

\[
   v = \frac{1}{3}(2V - U) = \frac{1}{3}(2)(2U - 3u) - U
\]

or

\[
   U = v + 2u
\]

And, solving for v from Equation 3.3c leads to

\[
   v = u + t
\]

which, when substituted into the above expression for U yields

\[
   U = v + 2u = u + t + 2u = u + t
\]

In solving for an expression for V, we begin with the one of the above expressions for this parameter—i.e.,

\[
   V = 2U - 3u
\]

Now, substitution of the above expression for U into this equation leads to

\[
   V = 2U - 3u = (2)(u + t) - 3u = u + 2t
\]
And solving for $u$ from Equation 3.3c gives

$$ u = v \quad t $$

which, when substituted in the previous equation results in the following expression for $V$

$$ V = u \quad 2t = (v \quad t) \quad 2t = v \quad t $$

And, of course from Equation 3.3d

$$ W = w $$
Crystallographic Planes

3.20 (a) Draw an orthorhombic unit cell, and within that cell a (210) plane.

(b) Draw a monoclinic unit cell, and within that cell a (002) plane.

Solution

(a) We are asked to draw a (210) plane within an orthorhombic unit cell. First remove the three indices from the parentheses, and take their reciprocals—i.e., 1/2, 1, and ∞. This means that the plane intercepts the x-axis at a/2, the y-axis at b, and parallels the z-axis. The plane that satisfies these requirements has been drawn within the orthorhombic unit cell below. (For orthorhombic, \(a \neq b \neq c\), and \(\alpha = \beta = \gamma = 90^\circ\).)

(b) A (002) plane is drawn within the monoclinic cell shown below. We first remove the parentheses and take the reciprocals of the indices; this gives \(\infty, \infty, \text{ and } 1/2\). Thus, the (002) plane parallels both x- and y-axes, and intercepts the z-axis at a/2, as indicated in the drawing. (For monoclinic, \(a \neq b \neq c\), and \(\alpha = \gamma = 90^\circ \neq \beta\).)
### 3.21 What are the indices for the two planes drawn in the sketch below?

![Sketch of two planes](image)

**Solution**

Plane 1 is a (020) plane. The determination of its indices is summarized below.

<table>
<thead>
<tr>
<th>( x )</th>
<th>( y )</th>
<th>( z )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \infty )</td>
<td>( a )</td>
<td>( b/2 )</td>
</tr>
<tr>
<td>Intercepts in terms of ( a ), ( b ), and ( c )</td>
<td>( \infty )</td>
<td>( 1/2 )</td>
</tr>
<tr>
<td>Reciprocals of intercepts</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td>Enclosure</td>
<td>(020)</td>
<td></td>
</tr>
</tbody>
</table>

Plane 2 is a \((2\overline{2}1)\) plane, as summarized below.

<table>
<thead>
<tr>
<th>( x )</th>
<th>( y )</th>
<th>( z )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a/2 )</td>
<td>(-b/2)</td>
<td>( c )</td>
</tr>
<tr>
<td>Intercepts in terms of ( a ), ( b ), and ( c )</td>
<td>( 1/2 )</td>
<td>(-1/2)</td>
</tr>
<tr>
<td>Reciprocals of intercepts</td>
<td>2</td>
<td>-2</td>
</tr>
<tr>
<td>Enclosure</td>
<td>(2\overline{2}1)</td>
<td></td>
</tr>
</tbody>
</table>
3.22 Sketch within a cubic unit cell the following planes:

(a) (011), (e) (111),
(b) (112), (f) (122),
(c) (102), (g) (123),
(d) (131), (h) (013)

Solution

The planes called for are plotted in the cubic unit cells shown below.
3.23 Determine the Miller indices for the planes shown in the following unit cell:

Solution

For plane A we will leave the origin at the unit cell as shown; this is a \((403)\) plane, as summarized below.

<table>
<thead>
<tr>
<th>(x)</th>
<th>(y)</th>
<th>(z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\frac{a}{2})</td>
<td>(\infty b)</td>
<td>(\frac{2c}{3})</td>
</tr>
<tr>
<td>Intercepts in terms of (a, b,) and (c)</td>
<td>(\frac{1}{2})</td>
<td>(\infty)</td>
</tr>
<tr>
<td>Reciprocals of intercepts</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>Reduction</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>Enclosure</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

For plane B we will move the origin of the unit cell one unit cell distance to the right along the \(y\) axis, and one unit cell distance parallel to the \(x\) axis; thus, this is a \((\bar{1} \bar{1} 2)\) plane, as summarized below.

<table>
<thead>
<tr>
<th>(x)</th>
<th>(y)</th>
<th>(z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(-a)</td>
<td>(-b)</td>
<td>(\frac{c}{2})</td>
</tr>
<tr>
<td>Intercepts in terms of (a, b,) and (c)</td>
<td>(-1)</td>
<td>(-1)</td>
</tr>
<tr>
<td>Reciprocals of intercepts</td>
<td>(-1)</td>
<td>(-1)</td>
</tr>
<tr>
<td>Reduction</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Enclosure</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
3.24 Determine the Miller indices for the planes shown in the following unit cell:

Solution

For plane A we will move the origin of the coordinate system one unit cell distance to the upward along the z axis; thus, this is a (322) plane, as summarized below.

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>a/3</td>
<td>b/2</td>
<td>-c/2</td>
</tr>
</tbody>
</table>

Intercepts in terms of a, b, and c

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/3</td>
<td>1/2</td>
<td>-1/2</td>
</tr>
</tbody>
</table>

Reciprocals of intercepts

3 2 -2

Reduction (not necessary)

Enclosure (322)

For plane B we will move the origin of the coordinate system one unit cell distance along the x axis; thus, this is a (101) plane, as summarized below.

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>-a/2</td>
<td>b</td>
<td>c/2</td>
</tr>
</tbody>
</table>

Intercepts in terms of a, b, and c

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1/2</td>
<td>1</td>
<td>1/2</td>
</tr>
</tbody>
</table>

Reciprocals of intercepts

-2 0 2

Reduction -1 0 1

Enclosure (101)
3.25 Determine the Miller indices for the planes shown in the following unit cell:

![Unit Cell Diagram](image)

**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 to the right along the y axis; thus, this is a \((\frac{3}{2}24)\) plane, as summarized below.

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\frac{2a}{3})</td>
<td>(-b)</td>
<td>(\frac{c}{2})</td>
</tr>
</tbody>
</table>

Intercepts in terms of \(a\), \(b\), and \(c\)

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\frac{2}{3})</td>
<td>(-1)</td>
<td>(\frac{1}{2})</td>
</tr>
</tbody>
</table>

Reciprocals of intercepts

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\frac{3}{2})</td>
<td>(-1)</td>
<td>2</td>
</tr>
</tbody>
</table>

Reduction

\[3 - 2\]

Enclosure

\((\frac{3}{2}24)\)

For plane B we will leave the origin at the unit cell as shown; this is a \((221)\) plane, as summarized below.

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>(b)</td>
<td>(c)</td>
</tr>
</tbody>
</table>

Intercepts in terms of \(a\), \(b\), and \(c\)

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\frac{1}{2})</td>
<td>(\frac{1}{2})</td>
<td>1</td>
</tr>
</tbody>
</table>

Reciprocals of intercepts

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
</tbody>
</table>

Reduction

not necessary

Enclosure

\((221)\)
3.26 Cite the indices of the direction that results from the intersection of each of the following pair of planes within a cubic crystal: (a) (100) and (010) planes, (b) (111) and (11̅1) planes, and (c) (10̅1) and (001) planes.

Solution

(a) In the figure below is shown (100) and (010) planes, and, as indicated, their intersection results in a [001], or equivalently, a [001] direction.

(b) In the figure below is shown (111) and (11̅1) planes, and, as indicated, their intersection results in a [1̅10], or equivalently, a [1̅10] direction.
(c) In the figure below is shown $(10\bar{1})$ and (001) planes, and, as indicated, their intersection results in a [010], or equivalently, a $[\bar{1}0\bar{1}]$ direction.
3.27 Convert the (010) and (101) planes into the four-index Miller–Bravais scheme for hexagonal unit cells.

**Solution**

For (010), \( h = 0 \), \( k = 1 \), and \( l = 0 \), and, from Equation 3.6, the value of \( i \) is equal to

\[
i = (h + k) = (0 + 1) = 1
\]

Therefore, the (010) plane becomes \((01\bar{1}0)\).

Now for the (101) plane, \( h = 1 \), \( k = 0 \), and \( l = 1 \), and computation of \( i \) using Equation 3.6 leads to

\[
i = (h + k) = [1 + 0] = 1
\]

such that (101) becomes \((10\bar{1}1)\).
3.28 Determine the indices for the planes shown in the following hexagonal unit cells:

Solution

(a) For this plane, intersections with the $a_1$, $a_2$, and $z$ axes are $\infty a$, $\infty a$, and $c/2$ (the plane parallels both $a_1$ and $a_2$ axes). In terms of $a$ and $c$ these intersections are $\infty$, $\infty$, and $\frac{1}{2}$, the respective reciprocals of which are 0, 0, and 2. This means that

$$h = 0$$
$$k = 0$$
$$l = 2$$

Now, from Equation 3.6, the value of $i$ is

$$i = (h + k) = [0 + 0] = 0$$

Hence, this is a (0002) plane.
(b) This plane passes through the origin of the coordinate axis system; therefore, we translate this plane one unit distance along the \(x\) axis, per the sketch shown below:

At this point the plane intersects the \(a_1\), \(a_2\), and \(z\) axes at \(a, \infty a,\) and \(\infty c\), respectively (the plane parallels both \(a_2\) and \(z\) axes). In terms of \(a\) and \(c\) these intersections are 1, \(\infty,\) and \(\infty,\) the respective reciprocals of which are 1, 0, and 0. This means that
\[
\begin{align*}
h &= 1 \\
k &= 0 \\
l &= 0
\end{align*}
\]
Now, from Equation 3.6, the value of \(i\) is
\[
\begin{align*}
i &= (h + k) = (1 + 0) = 1
\end{align*}
\]
Hence, this is a \((1010)\) plane.
(c) For this plane, intersections with the $a_1$, $a_2$, and $z$ axes are $-a$, $a$, and $c$. In terms of $a$ and $c$ these intersections are $-1$, 1, and 1, the respective reciprocals of which are 0, 1, and 1. This means that

$$h = -1$$
$$k = 1$$
$$l = 1$$

Now, from Equation 3.6, the value of $i$ is

$$i = (h + k) = (1 + 1) = 0$$

Hence, this is a $(\overline{1}101)$ plane.

(d) For this plane, intersections with the $a_1$, $a_2$, and $z$ axes are $-a/2$, $a$, and $c/2$, respectively. In terms of $a$ and $c$ these intersections are $-1/2$, 1, and 1/2, the respective reciprocals of which are $-2$, 1, and 2. This means that

$$h = -2$$
$$k = 1$$
$$l = 2$$

Now, from Equation 3.6, the value of $i$ is

$$i = (h + k) = (2 + 1) = 1$$

Therefore, this is a $(\overline{2}112)$ plane.
3.29 Sketch the \( \{1\bar{1}01\} \) and \( \{11\bar{2}0\} \) planes in a hexagonal unit cell.

**Solution**

For \( \{1\bar{1}01\} \) the reciprocals of \( h, k, i \), and \( l \) are, respectively, 1, \(-1\), \(\infty\), and 1; thus, this plane is parallel to the \( a_3 \) axis, and intersects the \( a_1 \) axis at \( a \), the \( a_2 \) axis at \(-a\), and the \( z \)-axis at \( c \). The plane having these intersections is shown in the figure below.

For \( \{11\bar{2}0\} \) the reciprocals of \( h, k, i \), and \( l \) are, respectively, 1, 1, \(-1/2\), and \(\infty\); thus, this plane is parallel to the \( z \) axis, and intersects the \( a_1 \) axis at \( a \), the \( a_2 \) axis at \( a \), and the \( a_3 \) axis at \(-a/2\). The plane having these intersections is shown in the figure below.
Polycrystalline Materials

3.30 Explain why the properties of polycrystalline materials are most often isotropic.

Solution

Although each individual grain in a polycrystalline material may be anisotropic, if the grains have random orientations, then the solid aggregate of the many anisotropic grains will behave isotropically.
Noncrystalline Solids

3.31 Would you expect a material in which the atomic bonding is predominantly ionic in nature to be more or less likely to form a noncrystalline solid upon solidification than a covalent material? Why? (See Section 2.6.)

Solution

A material in which atomic bonding is predominantly ionic in nature is less likely to form a noncrystalline solid upon solidification than a covalent material because covalent bonds are directional whereas ionic bonds are nondirectional; it is more difficult for the atoms in a covalent material to assume positions giving rise to an ordered structure.