Repeat distance  The distance from one lattice point to the adjacent lattice point along a direction.
Short-range order  The regular and predictable arrangement of the atoms over a short distance—usually one or two atom spacings.
Stacking sequence  The sequence in which close-packed planes are stacked. If the sequence is \textit{ABABAB}, a hexagonal close-packed unit cell is produced; if the sequence is \textit{ABCABCABC}, a face-centered cubic structure is produced.
Stress-induced crystallization  The process of forming crystals by the application of an external stress. Typically, a significant fraction of many amorphous plastics can be crystallized in this fashion, making them stronger.
Tetrahedral site  An interstitial position that has a coordination number of four. An atom or ion in the tetrahedral site has four nearest neighbor atoms or ions.
Tetrahedron  The structure produced when atoms are packed together with a four-fold coordination.
Transmission electron microscopy (TEM)  A technique for imaging and analysis of microstructures using a high energy electron beam.
Unit cell  A subdivision of the lattice that still retains the overall characteristics of the entire lattice.
X-ray diffraction (XRD)  A technique for analysis of crystalline materials using a beam of x-rays.

Problems

Section 3-1 Short-Range Order versus Long-Range Order

3-1 What is a “crystalline” material?
3-2 What is a single crystal?
3-3 State any two applications where single crystals are used.
3-4 What is a polycrystalline material?
3-5 What is a liquid crystal material?
3-6 What is an amorphous material?
3-7 Why do some materials assume an amorphous structure?
3-8 State any two applications of amorphous silicate glasses.

Section 3-2 Amorphous Materials: Principles and Technological Applications

3-9 What is meant by the term glass-ceramic?
3-10 Briefly compare the mechanical properties of glasses and glass-ceramics.

Section 3-3 Lattice, Unit Cells, Basis, and Crystal Structures

3-11 Define the terms lattice, unit cell, basis, and crystal structure.
3-12 Explain why there is no face-centered tetragonal Bravais lattice.
3-13 Calculate the atomic radius in cm for the following:
   (a) BCC metal with \(a_0 = 0.3294 \text{ nm}\); and
   (b) FCC metal with \(a_0 = 4.0862 \text{ Å}\).
3-14 Determine the crystal structure for the following:
   (a) a metal with \(a_0 = 4.9489 \text{ Å}, r = 1.75 \text{ Å}\), and one atom per lattice point; and
   (b) a metal with \(a_0 = 0.42906 \text{ nm}, r = 0.1858 \text{ nm}\), and one atom per lattice point.
3-15 The density of potassium, which has the BCC structure, is 0.855 \text{ g/cm}^3. The atomic weight of potassium is 39.09 \text{ g/mol}. Calculate (a) the lattice parameter; and (b) the atomic radius of potassium.
3-16 The density of thorium, which has the FCC structure, is 11.72 \text{ g/cm}^3. The atomic weight of thorium is 232 \text{ g/mol}. Calculate (a) the lattice parameter; and (b) the atomic radius of thorium.
3-17 A metal having a cubic structure has a density of 2.6 \text{ g/cm}^3, an atomic weight of 87.62 \text{ g/mol}, and a lattice parameter of 6.0849 \text{ Å}. One atom is associated with each lattice point. Determine the crystal structure of the metal.
3-18 A metal having a cubic structure has a density of 1.892 \text{ g/cm}^3, an atomic weight of
132.91 g/mol, and a lattice parameter of 6.13 Å. One atom is associated with each lattice point. Determine the crystal structure of the metal.

3-19 Indium has a tetragonal structure, with \( a_0 = 0.32517 \text{ nm} \) and \( c_0 = 0.49459 \text{ nm} \). The density is 7.286 g/cm\(^3\), and the atomic weight is 114.82 g/mol. Does indium have the simple tetragonal or body-centered tetragonal structure?

3-20 Bismuth has a hexagonal structure, with \( a_0 = 0.4546 \text{ nm} \) and \( c_0 = 1.186 \text{ nm} \). The density is 9.808 g/cm\(^3\), and the atomic weight is 208.98 g/mol. Determine
(a) the volume of the unit cell; and
(b) the number of atoms in each unit cell.

3-21 Gallium has an orthorhombic structure, with \( a_0 = 0.45258 \text{ nm} \), \( b_0 = 0.45186 \text{ nm} \), and \( c_0 = 0.76570 \text{ nm} \). The atomic radius is 0.1143 nm, the density is 5.904 g/cm\(^3\), and the atomic weight is 69.72 g/mol. Determine
(a) the number of atoms in each unit cell; and
(b) the packing factor in the unit cell.

3-22 Beryllium has a hexagonal crystal structure, with \( a_0 = 0.22858 \text{ nm} \) and \( c_0 = 0.35842 \text{ nm} \). The atomic radius is 0.1218 nm. The density is 1.848 g/cm\(^3\), and the atomic weight is 9.01 g/mol. Determine
(a) the number of atoms in each unit cell; and
(b) the packing factor in the unit cell.

3-23 A typical paper clip weighs 0.59 g and consists of BCC iron. Calculate
(a) the number of unit cells; and
(b) the number of iron atoms in the paper clip. (See Appendix A for required data.)

3-24 Aluminum foil used to package food is approximately 0.001 inch thick. Assume that all of the unit cells of the aluminum are arranged so that \( a_0 \) is perpendicular to the foil surface. For a 4 in. \( \times \) 4 in. square of the foil, determine
(a) the total number of unit cells in the foil; and
(b) the thickness of the foil in number of unit cells. (See Appendix A.)

3-25 Rutile is the name given to a crystal structure commonly adopted by compounds of the form AB\(_2\), where A represents a metal atom and B represents oxygen atoms. One form of rutile has atoms of element A at the unit cell coordinates \((0, 0, 0)\) and \((1/2, 1/2, 1/2)\) and atoms of element B at \((1/4, 1/4, 0), (3/4, 3/4, 0), (3/4, 1/4, 1/2), \) and \((1/4, 3/4, 1/2)\). The unit cell parameters are \( a = b \neq c \) and \( \alpha = \beta = \gamma = 90^\circ \). Note that the lattice parameter \( c \) is typically smaller than the lattice parameters \( a \) and \( b \) for the rutile structure.

(a) How many atoms of element A are there per unit cell?
(b) How many atoms of element B are there per unit cell?
(c) Is your answer to part (b) consistent with the stoichiometry of an AB\(_2\) compound? Explain.
(d) Draw the unit cell for rutile. Use a different symbol for each type of atom. Provide a legend indicating which symbol represents which type of atom.
(e) For the simple tetragonal lattice, \( a = b \neq c \) and \( \alpha = \beta = \gamma = 90^\circ \). There is one lattice point per unit cell located at the corners of the simple tetragonal lattice. Describe the rutile structure as a simple tetragonal lattice and a basis.

3-26 Consider the CuAu crystal structure. It can be described as a simple cubic lattice with a basis of Cu \((0, 0, 0)\), Cu \((1/2, 1/2, 0)\), Au \((1/2, 0, 1/2)\), and Au \((0, 1/2, 1/2)\).

(a) How many atoms of each type are there per unit cell?
(b) Draw the unit cell for CuAu. Use a different symbol for each type of atom. Provide a legend indicating which symbol represents which type of atom.
(c) Give an alternative lattice and basis representation for CuAu for which one atom of the basis is Au \((0, 0, 0)\).
(d) A related crystal structure is that of Cu\(_3\)Au. This unit cell is similar to the face-centered cubic unit cell with Au at the corners of the unit cell and Cu at all of the face-centered positions. Describe this structure as a lattice and a basis.
(e) The Cu\(_3\)Au crystal structure is similar to the FCC crystal structure, but it does not have the face-centered cubic lattice. Explain briefly why this is the case.

3-27 Nanowires are high aspect-ratio metal or semiconducting wires with diameters on the
order of 1 to 100 nanometers and typical lengths of 1 to 100 microns. Nanowires likely will be used in the future to create high-density electronic circuits.

Nanowires can be fabricated from ZnO. ZnO has the wurtzite structure. The wurtzite structure is a hexagonal lattice with four atoms per lattice point at Zn (0, 0, 0), Zn (2/3, 1/3, 1/2), O (0, 0, 3/8), and O (2/3, 1/3, 7/8).

(a) How many atoms are there in the conventional unit cell?

(b) If the atoms were located instead at Zn (0, 0, 0), Zn (1/3, 2/3, 1/2), O (0, 0, 3/8), and O (1/3, 2/3, 7/8), would the structure be different? Please explain.

(c) For ZnO, the unit cell parameters are \( a = 3.24 \text{ Å} \) and \( c = 5.19 \text{ Å} \). (Note: This is not the ideal HCP \( c/a \) ratio.) A typical ZnO nanowire is 20 nm in diameter and 5 \( \mu \text{m} \) long. Assume that the nanowires are cylindrical. Approximately how many atoms are there in a single ZnO nanowire?

3-28 Calculate the atomic packing fraction for the hexagonal close-packed crystal structure for which \( c = \frac{8}{3} a \). Remember that the base of the unit cell is a parallelogram.

**Section 3-4 Allotropic or Polymorphic Transformations**

3-29 What is the difference between an allotrope and a polymorph?

3-30 What are the different polymorphs of zirconia?

3-31 Above 882°C, titanium has a BCC crystal structure, with \( a = 0.332 \text{ nm} \). Below this temperature, titanium has a HCP structure with \( a = 0.2978 \text{ nm} \) and \( c = 0.4735 \text{ nm} \). Determine the percent volume change when BCC titanium transforms to HCP titanium. Is this a contraction or expansion?

3-32 \( \alpha \)-Mn has a cubic structure with \( a_0 = 0.8931 \text{ nm} \) and a density of 7.47 g/cm\(^3\). \( \beta \)-Mn has a different cubic structure with \( a_0 = 0.6326 \text{ nm} \) and a density of 7.26 g/cm\(^3\). The atomic weight of manganese is 54.938 g/mol and the atomic radius is 0.112 nm. Determine the percent volume change that would occur if \( \alpha \)-Mn transforms to \( \beta \)-Mn.

3-33 Calculate the theoretical density of the three polymorphs of zirconia. The lattice constants for the monoclinic form are \( a = 5.156, \ b = 5.191, \) and \( c = 5.304 \text{ Å} \), respectively. The angle \( \beta \) for the monoclinic unit cell is 98.9°. The lattice constants for the tetragonal unit cell are \( a = 5.094 \) and \( c = 5.304 \text{ Å} \), respectively. Cubic zirconia has a lattice constant of 5.124 Å.

3-34 From the information in this chapter, calculate the volume change that will occur when the cubic form of zirconia transforms into a tetragonal form.

3-35 Monoclinic zirconia cannot be used effectively for manufacturing oxygen sensors or other devices. Explain.

3-36 What is meant by the term stabilized zirconia?

3-37 State any two applications of stabilized zirconia ceramics.

**Section 3-5 Points, Directions, and Planes in the Unit Cell**

3-38 Explain the significance of crystallographic directions using an example of an application.

3-39 Why are Fe-Si alloys used in magnetic applications “grain oriented?”

3-40 How is the influence of crystallographic direction on magnetic properties used in magnetic materials for recording media applications?

3-41 Determine the Miller indices for the directions in the cubic unit cell shown in Figure 3-39.
3-42 Determine the indices for the directions in the cubic unit cell shown in Figure 3-40.

Figure 3-40 Directions in a cubic unit cell for Problem 3-42.

3-43 Determine the indices for the planes in the cubic unit cell shown in Figure 3-41.

Figure 3-41 Planes in a cubic unit cell for Problem 3-43.

3-44 Determine the indices for the planes in the cubic unit cell shown in Figure 3-42.

Figure 3-42 Planes in a cubic unit cell for Problem 3-44.

3-45 Determine the indices for the directions in the hexagonal lattice shown in Figure 3-43, using both the three-digit and four-digit systems.

Figure 3-43 Directions in a hexagonal lattice for Problem 3-45.

3-46 Determine the indices for the directions in the hexagonal lattice shown in Figure 3-44, using both the three-digit and four-digit systems.

Figure 3-44 Directions in a hexagonal lattice for Problem 3-46.
3-47 Determine the indices for the planes in the hexagonal lattice shown in Figure 3-45.

3-48 Determine the indices for the planes in the hexagonal lattice shown in Figure 3-46.

3-49 Sketch the following planes and directions within a cubic unit cell:
(a) [101] (b) [010] (c) [122] (d) [301] (e) [201] (f) [213] (g) [011] (h) [102] (i) [002] (j) [130] (k) [212] (l) [312]

3-50 Sketch the following planes and directions within a cubic unit cell:
(a) [110] (b) [221] (c) [410] (d) [012] (e) [321] (f) [111] (g) [111] (h) [011] (i) [030] (j) [121] (k) [113] (l) [041]

3-51 Sketch the following planes and directions within a hexagonal unit cell:
(a) [010] (b) [110] (c) [011] (d) (003) (e) (101) (f) (011)

3-52 Sketch the following planes and directions within a hexagonal unit cell:
(a) [2110] (b) [1111] (c) [0100] (d) (1210) (e) (1122) (f) (1230)

3-53 What are the indices of the six directions of the form (110) that lie in the (111) plane of a cubic cell?

3-54 What are the indices of the four directions of the form (111) that lie in the (101) plane of a cubic cell?

3-55 Determine the number of directions of the form (110) in a tetragonal unit cell and compare to the number of directions of the form (110) in an orthorhombic unit cell.

3-56 Determine the angle between the [110] direction and the (110) plane in a tetragonal unit cell; then determine the angle between the [011] direction and the (011) plane of a tetragonal cell. The lattice parameters are $a_0 = 4.0 \text{ Å}$ and $c_0 = 5.0 \text{ Å}$. What is responsible for the difference?

3-57 Determine the Miller indices of the plane that passes through three points having the following coordinates:
(a) 0, 0, 1; 1, 0, 0; and 1/2, 1/2, 0
(b) 1/2, 0, 1; 1/2, 0, 0; and 0, 1, 0
(c) 1, 0, 0; 0, 1, 1/2; and 1, 1/2, 1/4
(d) 1, 0, 0; 0, 0, 1/4; and 1/2, 1, 0

3-58 Determine the repeat distance, linear density, and packing fraction for FCC nickel, which has a lattice parameter of 0.35167 nm, in the [100], [110], and [111] directions. Which of these directions is close packed?

3-59 Determine the repeat distance, linear density, and packing fraction for BCC lithium, which has a lattice parameter of 0.35089 nm, in the [100], [110], and [111] directions. Which of these directions is close packed?

3-60 Determine the repeat distance, linear density, and packing fraction for HCP magnesium in the [2110] direction and the [1120] direction. The lattice parameters for HCP magnesium are given in Appendix A.