QUESTIONS AND PROBLEMS

Fundamental Concepts

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

Unit Cells
Metallic Crystal Structures

3.2 If the atomic radius of lead is 0.175 nm, calculate the volume of its unit cell in cubic meters.

3.3 Show for the body-centered cubic crystal structure that the unit cell edge length a and the atomic radius R are related through $a = 4R/\sqrt{3}$.

3.4 For the HCP crystal structure, show that the ideal c/a ratio is 1.633.

3.5 Show that the atomic packing factor for BCC is 0.68.

3.6 Show that the atomic packing factor for HCP is 0.74.

Density Computations

3.7 Molybdenum has a BCC crystal structure, an atomic radius of 0.1363 nm, and an atomic weight of 95.94 g/mol. Compute and compare its theoretical density with the experimental value found inside the front cover.

3.8 Calculate the radius of a palladium atom, given that Pd has an FCC crystal structure, a density of 12.0 g/cm^3, and an atomic weight of 106.4 g/mol.

3.9 Calculate the radius of a tantalum atom, given that Ta has a BCC crystal structure, a density of 16.6 g/cm^3, and an atomic weight of 180.9 g/mol.

3.10 Some hypothetical metal has the simple cubic crystal structure shown in Figure 3.23. If its atomic weight is 74.5 g/mol and the atomic radius is 0.145 nm, compute its density.

3.11 Titanium has an HCP crystal structure and a density of 4.51 g/cm^3.

(a) What is the volume of its unit cell in cubic meters?

(b) If the c/a ratio is 1.58, compute the values of c and a.

3.12 Using atomic weight, crystal structure, and atomic radius data tabulated inside the front cover, compute the theoretical densities of aluminum, nickel, magnesium, and tungsten, and then compare these values with the measured densities listed in this same table. The c/a ratio for magnesium is 1.624.

3.13 Niobium has an atomic radius of 0.1430 nm and a density of 8.57 g/cm^3. Determine whether it has an FCC or BCC crystal structure.

3.14 Below are listed the atomic weight, density, and atomic radius for three hypothetical alloys. For each determine whether its crystal structure is FCC, BCC, or simple cubic and then justify your determination. A simple cubic unit cell is shown in Figure 3.23.

Alloy	*Atomic Weight (g/mol)*	*Density (g/cm^3)*	*Atomic Radius (nm)*
A	43.1	6.40	0.122
B	184.4	12.30	0.146
C	91.6	9.60	0.137

3.15 The unit cell for uranium has orthorhombic symmetry, with a, b, and c lattice parameters of 0.286, 0.587, and 0.495 nm, respectively. If its density, atomic weight, and atomic radius are 19.05 g/cm^3, 238.03 g/mol, and 0.1385 nm, respectively, compute the atomic packing factor.

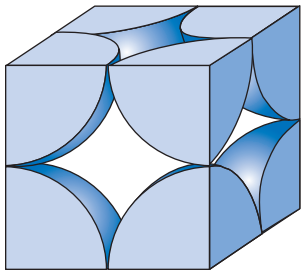


Figure 3.23 Hard-sphere unit cell representation of the simple cubic crystal structure.

3.16 Indium has a tetragonal unit cell for which the a and c lattice parameters are 0.459 and 0.495 nm, respectively.

(a) If the atomic packing factor and atomic radius are 0.693 and 0.1625 nm, respectively, determine the number of atoms in each unit cell.

(b) The atomic weight of indium is 114.82 g/mol; compute its theoretical density.

3.17 Beryllium has an HCP unit cell for which the ratio of the lattice parameters c/a is 1.568. If the radius of the Be atom is 0.1143 nm, **(a)** determine the unit cell volume, and **(b)** calculate the theoretical density of Be and compare it with the literature value.

3.18 Magnesium has an HCP crystal structure, a c/a ratio of 1.624, and a density of 1.74 g/cm^3. Compute the atomic radius for Mg.

3.19 Cobalt has an HCP crystal structure, an atomic radius of 0.1253 nm, and a c/a ratio of 1.623. Compute the volume of the unit cell for Co.

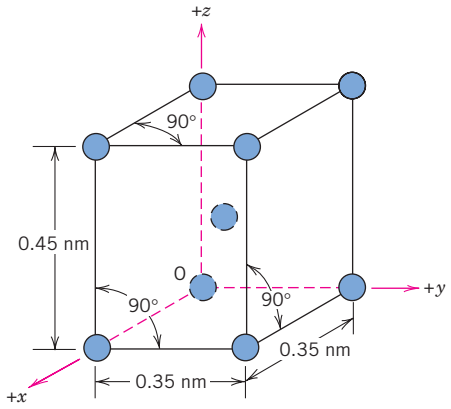
Crystal Systems

3.20 Below is 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 141 g/mol.



3.21 Sketch a unit cell for the face-centered orthorhombic crystal structure.

Point Coordinates

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

3.23 List the point coordinates of both the sodium and chlorine ions for a unit cell of the sodium chloride crystal structure (Figure 12.2).

3.24 List the point coordinates of both the zinc and sulfur atoms for a unit cell of the zinc blende crystal structure (Figure 12.4).

3.25 Sketch a tetragonal unit cell, and within that cell indicate locations of the $1\ 1\ \frac{1}{2}$ and $\frac{1}{2}\ \frac{1}{4}\ \frac{1}{2}$ point coordinates.

3.26 Using the Molecule Definition Utility found in both "Metallic Crystal Structures and Crystallography" and "Ceramic Crystal Structures" modules of *VMSE,* located on the book's web site [www.wiley.com/college/callister (Student Companion Site)], generate (and print out) a three-dimensional unit cell for β tin given the following: (1) the unit cell is tetragonal with $a = 0.583$ nm and $c = 0.318$ nm, and (2) Sn atoms are located at the following point coordinates:

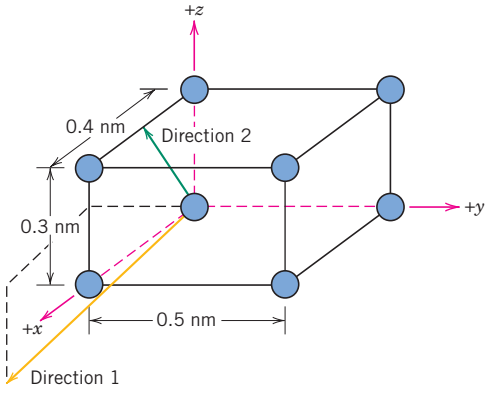
0 0 0	0 1 1
1 0 0	$\frac{1}{2}\ 0\ \frac{3}{4}$
1 1 0	$\frac{1}{2}\ 1\ \frac{3}{4}$
0 1 0	$1\ \frac{1}{2}\ \frac{1}{4}$
0 0 1	$0\ \frac{1}{2}\ \frac{1}{4}$
1 0 1	$\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$
1 1 1	

Crystallographic Directions

3.27 Draw an orthorhombic unit cell, and within that cell a $[2\bar{1}1]$ direction.

3.28 Sketch a monoclinic unit cell, and within that cell a $[\bar{1}01]$ direction.

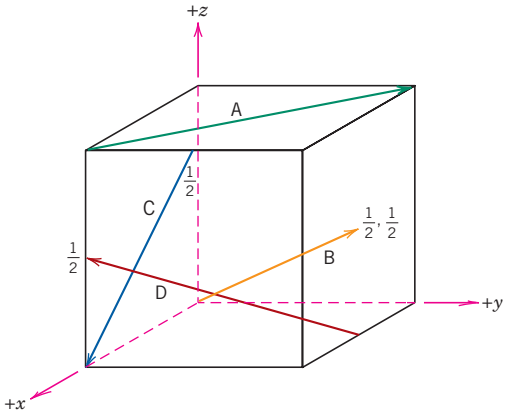
3.29 What are the indices for the directions indicated by the two vectors in the sketch below?



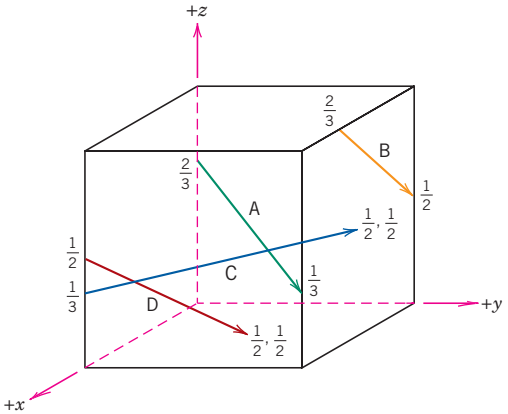
3.30 Within a cubic unit cell, sketch the following directions:

(a) [101], **(e)** $[\bar{1}1\bar{1}]$,
(b) [211], **(f)** $[\bar{2}12]$,
(c) $[10\bar{2}]$, **(g)** $[3\bar{1}2]$,
(d) $[3\bar{1}3]$, **(h)** [301].

3.31 Determine the indices for the directions shown in the following cubic unit cell:



3.32 Determine the indices for the directions shown in the following cubic unit cell:

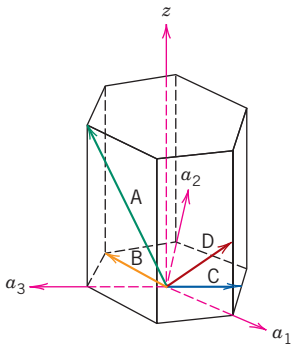


3.33 For tetragonal crystals, cite the indices of directions that are equivalent to each of the following directions:

(a) [011]
(b) [100]

3.34 Convert the [110] and $[00\bar{1}]$ directions into the four-index Miller–Bravais scheme for hexagonal unit cells.

3.35 Determine the indices for the directions shown in the following hexagonal unit cell:



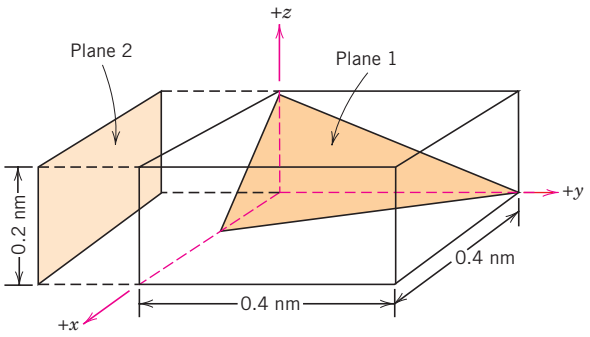
3.36 Using Equations 3.6a, 3.6b, 3.6c, and 3.6d, derive expressions for each of the three primed indices set (u', v', and w') in terms of the four unprimed indices (u, v, t, and w).

Crystallographic Planes

3.37 **(a)** Draw an orthorhombic unit cell, and within that cell a $(02\bar{1})$ plane.

(b) Draw a monoclinic unit cell, and within that cell a (200) plane.

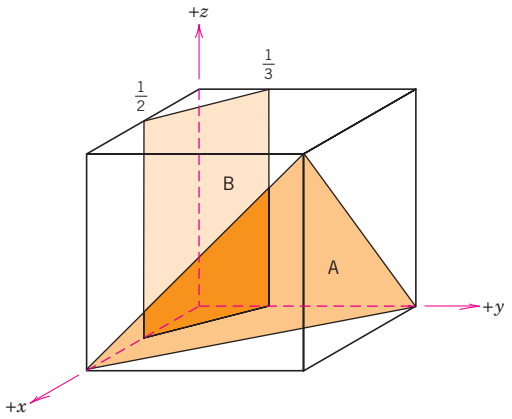
3.38 What are the indices for the two planes drawn in the sketch below?



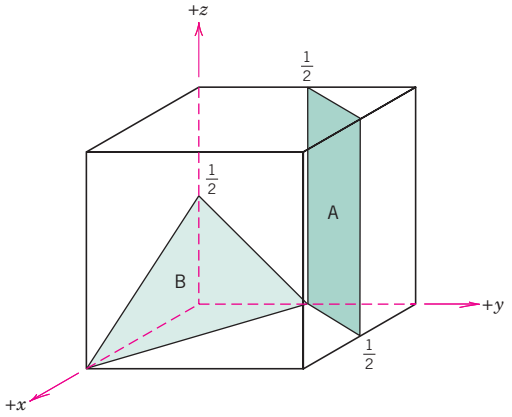
3.39 Sketch within a cubic unit cell the following planes:

(a) $(10\bar{1})$, **(e)** $(\bar{1}1\bar{1})$,
(b) $(2\bar{1}1)$, **(f)** $(\bar{2}12)$,
(c) (012), **(g)** $(3\bar{1}2)$,
(d) $(3\bar{1}3)$, **(h)** (301).

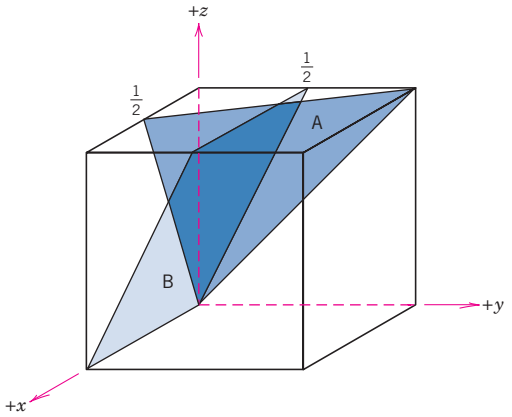
3.40 Determine the Miller indices for the planes shown in the following unit cell:



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



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



3.43 Cite the indices of the direction that results from the intersection of each of the following pair of planes within a cubic crystal: **(a)** (110) and (111) planes, **(b)** (110) and $(1\bar{1}0)$ planes, and **(c)** $(11\bar{1})$ and (001) planes.

3.44 Sketch the atomic packing of **(a)** the (100) plane for the FCC crystal structure, and **(b)** the (111) plane for the BCC crystal structure (similar to Figures 3.10*b* and 3.11*b*).

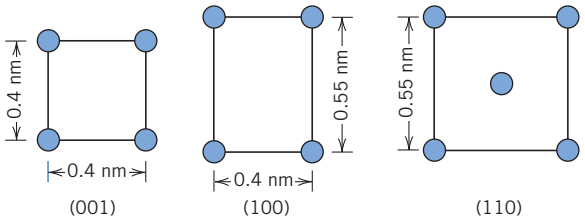
3.45 Consider the reduced-sphere unit cell shown in Problem 3.20, having an origin of the coordinate system positioned at the atom labeled with an O. For the following sets of planes, determine which are equivalent:

(a) (100), $(0\bar{1}0)$, and (001)

(b) (110), (101), (011), and $(\bar{1}01)$

(c) (111), $(1\bar{1}1)$, $(11\bar{1})$, and $(\bar{1}1\bar{1})$

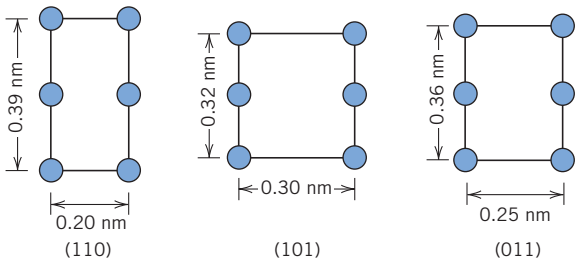
3.46 Here are three different crystallographic planes for a unit cell of a hypothetical metal. The circles represent atoms:



(a) To what crystal system does the unit cell belong?

(b) What would this crystal structure be called?

3.47 Below are shown three different crystallographic planes for a unit cell of some hypothetical metal. The circles represent atoms:



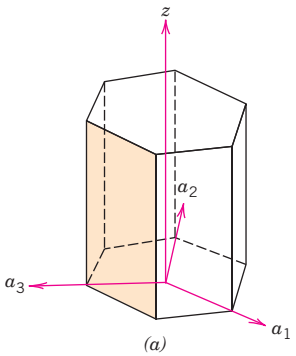
(a) To what crystal system does the unit cell belong?

(b) What would this crystal structure be called?

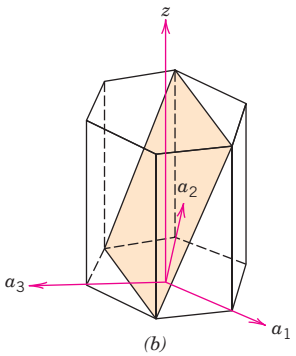
(c) If the density of this metal is 18.91 g/cm^3, determine its atomic weight.

3.48 Convert the (111) and $(0\bar{1}2)$ planes into the four-index Miller–Bravais scheme for hexagonal unit cells.

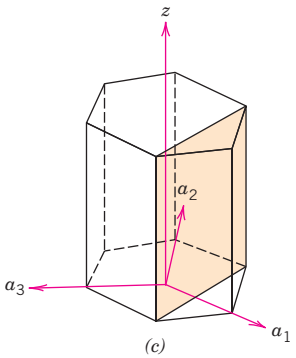
3.49 Determine the indices for the planes shown in the hexagonal unit cells below:



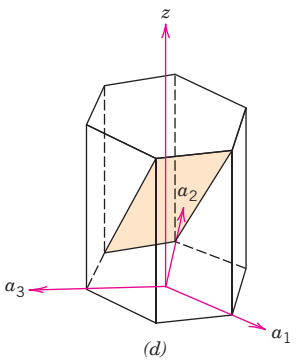
(a)



(b)



(c)



(d)

3.50 Sketch the $(01\bar{1}1)$ and $(2\bar{1}\bar{1}0)$ planes in a hexagonal unit cell.

Linear and Planar Densities

3.51 **(a)** Derive linear density expressions for FCC [100] and [111] directions in terms of the atomic radius R.

(b) Compute and compare linear density values for these same two planes for copper.

3.52 **(a)** Derive linear density expressions for BCC [110] and [111] directions in terms of the atomic radius R.

(b) Compute and compare linear density values for these same two planes for iron.

3.53 **(a)** Derive planar density expressions for FCC (100) and (111) planes in terms of the atomic radius R.

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

3.54 **(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.

3.55 **(a)** Derive the planar density expression for the HCP (0001) plane in terms of the atomic radius R.

(b) Compute the planar density value for this same plane for titanium.

Polycrystalline Materials

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

X-Ray Diffraction: Determination of Crystal Structures

3.57 Using the data for aluminum in Table 3.1, compute the interplanar spacing for the (110) set of planes.

3.58 Determine the expected diffraction angle for the first-order reflection from the (310) set of planes for BCC chromium when monochromatic radiation of wavelength 0.0711 nm is used.

3.59 Using the data for α-iron in Table 3.1, compute the interplanar spacings for the (111) and (211) sets of planes.

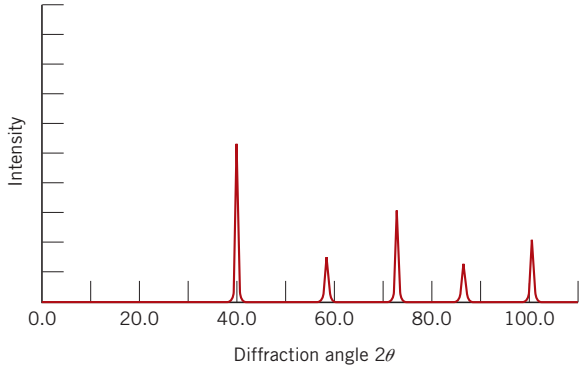


Figure 3.24 Diffraction pattern for powdered tungsten. (Courtesy of Wesley L. Holman.)

3.60 The metal rhodium has an FCC crystal structure. If the angle of diffraction for the (311) set of planes occurs at 36.12° (first-order reflection) when monochromatic x-radiation having a wavelength of 0.0711 nm is used, compute **(a)** the interplanar spacing for this set of planes, and **(b)** the atomic radius for a rhodium atom.

3.61 The metal niobium has a BCC crystal structure. If the angle of diffraction for the (211) set of planes occurs at 75.99° (first-order reflection) when monochromatic x-radiation having a wavelength of 0.1659 nm is used, compute **(a)** the interplanar spacing for this set of planes, and **(b)** the atomic radius for the niobium atom.

3.62 For which set of crystallographic planes will a first-order diffraction peak occur at a diffraction angle of 44.53° for FCC nickel when monochromatic radiation having a wavelength of 0.1542 nm is used?

3.63 Figure 3.21 shows an x-ray diffraction pattern for lead taken using a diffractometer and monochromatic x-radiation having a wavelength of 0.1542 nm; each diffraction peak on the pattern has been indexed. Compute the interplanar spacing for each set of planes indexed; also determine the lattice parameter of Pb for each of the peaks.

3.64 The diffraction peaks shown in Figure 3.21 are indexed according to the reflection rules for FCC (i.e., h, k, and l must all be either odd or even). Cite the h, k, and l indices of the first four diffraction peaks for BCC crystals consistent with $h + k + l$ being even.

3.65 Figure 3.24 shows the first five peaks of the x-ray diffraction pattern for tungsten, which has a BCC crystal structure; monochromatic x-radiation having a wavelength of 0.1542 nm was used.

(a) Index (i.e., give h, k, and l indices) for each of these peaks.

(b) Determine the interplanar spacing for each of the peaks.

(c) For each peak, determine the atomic radius for W and compare these with the value presented in Table 3.1.

Noncrystalline Solids

3.66 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.)