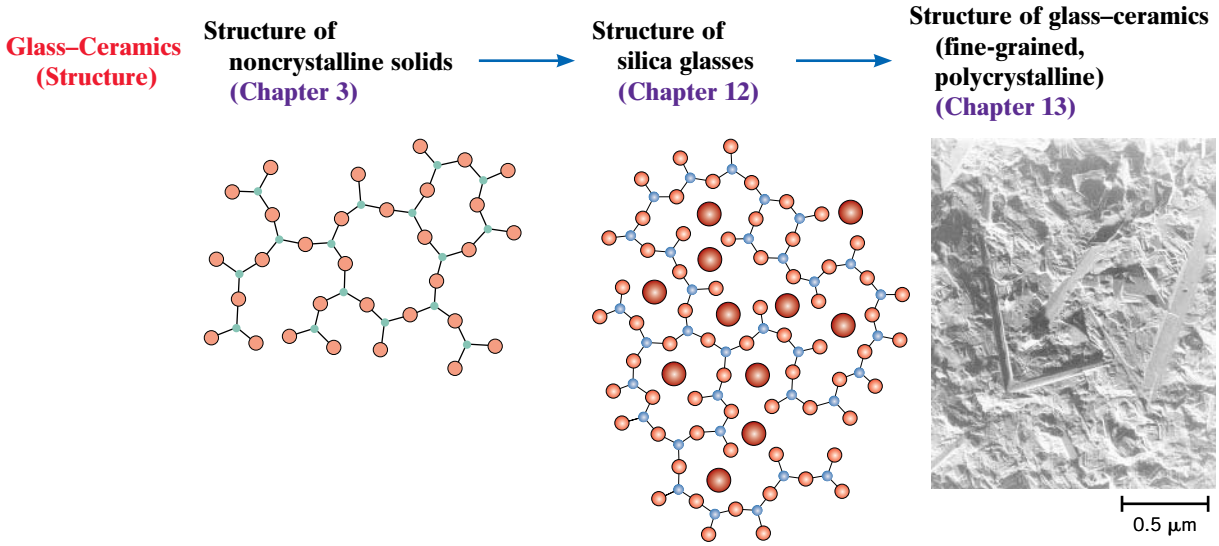
heat-treated so as to become crystalline in nature. The following concept map notes this relationship:



Important Terms and Concepts

allotropy
amorphous
anisotropy
atomic packing factor (APF)
body-centered cubic (BCC)
Bragg's law
coordination number
crystalline
crystal structure
crystal system
diffraction
face-centered cubic (FCC)
grain
grain boundary
hexagonal close-packed (HCP)
isotropic
lattice
lattice parameters
Miller indices
noncrystalline
polycrystalline
polymorphism
single crystal
unit cell

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QUESTIONS AND PROBLEMS

⊕ *Problem available (at instructor's discretion) in* WileyPLUS

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 struc- ⊕ ture 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 (Mo) 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 of the book.

3.8 Strontium (Sr) has an FCC crystal structure, an atomic radius of 0.215 nm, and an atomic weight of 87.62 g/mol. Calculate the theoretical density for Sr.

3.9 Calculate the radius of a palladium (Pd) 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.

3.10 Calculate the radius of a tantalum (Ta) 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.

3.11 A hypothetical metal has the simple cubic crystal structure shown in Figure 3.3. If its atomic weight is 74.5 g/mol and the atomic radius is 0.145 nm, compute its density.

3.12 Titanium (Ti) 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*.

3.13 Magnesium (Mg) has an HCP crystal structure and a density of 1.74 g/cm^3.

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

(b) If the *c/a* ratio is 1.624, compute the values of *c* and *a*.

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

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

3.16 The atomic weight, density, and atomic radius for three hypothetical alloys are listed in the following table. For each, determine whether its crystal structure is FCC, BCC, or simple cubic and then justify your determination.

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

3.17 The unit cell for uranium (U) 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.

3.18 Indium (In) 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 In is 114.82 g/mol; compute its theoretical density.

3.19 Beryllium (Be) 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.

3.20 Magnesium (Mg) 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.

3.21 Cobalt (Co) 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.

Polymorphism and Allotropy

3.22 Iron (Fe) undergoes an allotropic transformation at 912°C: upon heating from a BCC (α phase) to an FCC (γ phase). Accompanying this transformation is a change in the atomic radius of Fe—from R_{BCC} = 0.12584 nm to R_{FCC} = 0.12894 nm—and, in addition, a change in density (and volume). Compute the percentage volume change associated with this reaction. Does the volume increase or decrease?

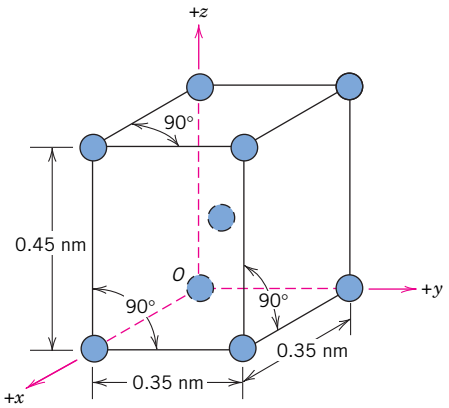
Crystal Systems

3.23 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 141 g/mol.



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

Point Coordinates

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

3.26 List the point coordinates of both the sodium (Na) and chlorine (Cl) ions for a unit cell of the NaCl crystal structure (Figure 12.2).

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

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

3.29 Sketch an orthorhombic unit cell, and within that cell indicate locations of the $0\,\frac{1}{2}\,1$ and $\frac{1}{3}\,\frac{1}{4}\,\frac{1}{4}$ point coordinates.

3.30 Using the Molecule Definition Utility found in the "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 (Sn), 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:

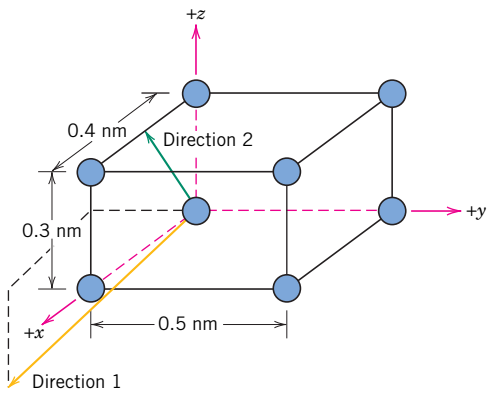
0 0 0	0 1 1
1 0 0	$\frac{1}{2}\,0\,\frac{3}{4}$
1 1 0	$\frac{1}{2}\,1\,\frac{3}{4}$
0 1 0	$1\,\frac{1}{2}\,\frac{1}{4}$
0 0 1	$0\,\frac{1}{2}\,\frac{1}{4}$
1 0 1	$\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$
1 1 1	

Crystallographic Directions

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

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

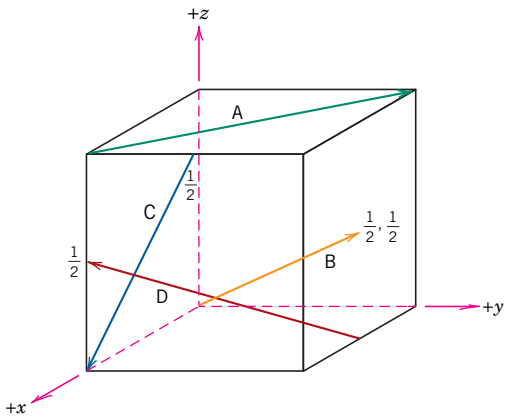
3.33 What are the indices for the directions indicated by the two vectors in the following sketch?



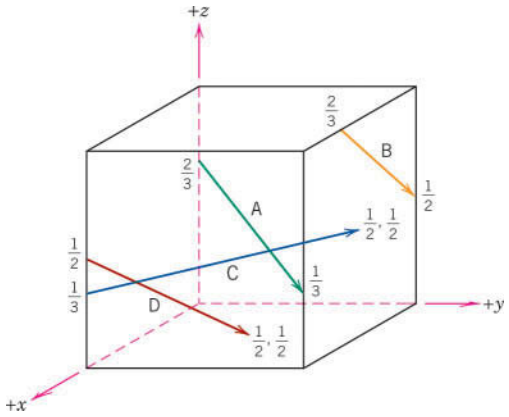
3.34 Within a cubic unit cell, sketch the following directions:

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

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



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



3.37 **(a)** What are the direction indices for a vector that passes from point $\frac{1}{4}\,0\,\frac{1}{2}$ to point $\frac{3}{4}\,\frac{1}{2}\,\frac{1}{2}$ in a cubic unit cell?

(b) Repeat part **(a)** for a monoclinic unit cell.

3.38 **(a)** What are the direction indices for a vector that passes from point $\frac{1}{3}\,\frac{1}{2}\,0$ to point $\frac{2}{3}\,\frac{3}{4}\,\frac{1}{2}$ in a tetragonal unit cell?

(b) Repeat part **(a)** for a rhombohedral unit cell.

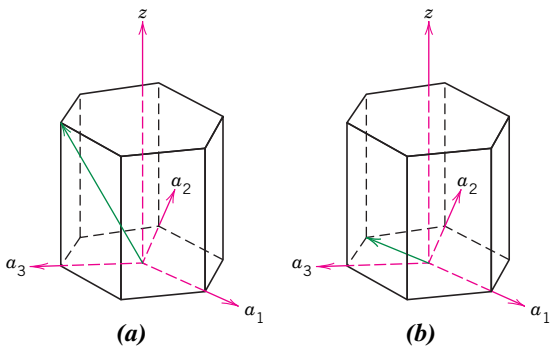
3.39 For tetragonal crystals, cite the indices of directions that are equivalent to each of the following directions:

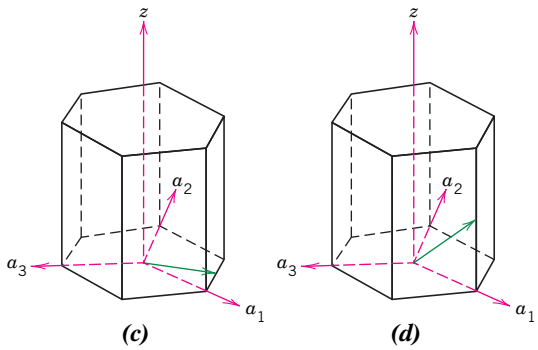
(a) [011]

(b) [100]

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

3.41 Determine the indices for the directions shown in the following hexagonal unit cells:





3.42 Sketch the $[01\bar{1}0]$ and $[\bar{2}\bar{2}43]$ directions in a hexagonal unit cell.

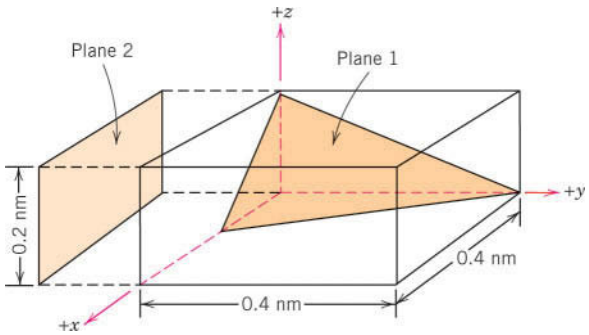
3.43 Using Equations 3.11a–3.11d, derive expressions for each of the three U, V, and W indices in terms of the four u, v, t, and w indices.

Crystallographic Planes

3.44 **(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.

3.45 What are the indices for the two planes drawn in the following sketch?



3.46 Sketch within a cubic unit cell the following planes:

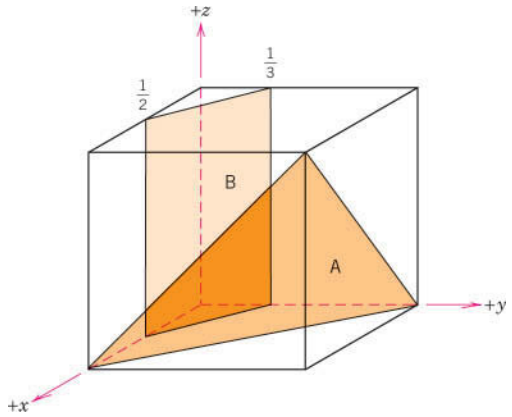
(a) $(10\bar{1})$ **(e)** $(\bar{1}1\bar{1})$

(b) $(2\bar{1}1)$ **(f)** $(\bar{2}12)$

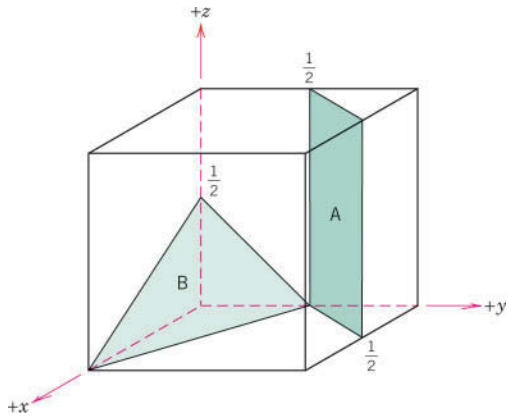
(c) (012) **(g)** $(3\bar{1}2)$

(d) $(3\bar{1}3)$ **(h)** (301)

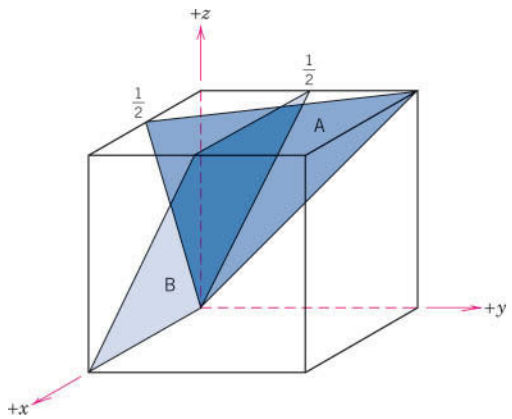
3.47 Determine the Miller indices for the planes shown in the following unit cell:



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



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



3.50 Cite the indices of the direction that results from the intersection of each of the following pairs of planes within a cubic crystal:

(a) The (110) and (111) planes

(b) The (110) and $(1\bar{1}0)$ planes

(c) The $(11\bar{1})$ and (001) planes

3.51 Sketch the atomic packing of the following:

(a) The (100) plane for the FCC crystal structure

(b) The (111) plane for the BCC crystal structure (similar to Figures 3.12*b* and 3.13*b*).

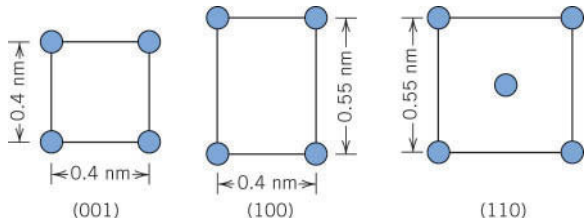
3.52 Consider the reduced-sphere unit cell shown in Problem 3.23, having an origin of the coordinate system positioned at the atom labeled *O*. For the following sets of planes, determine which are equivalent:

(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 $(\bar{1}1\bar{1})$

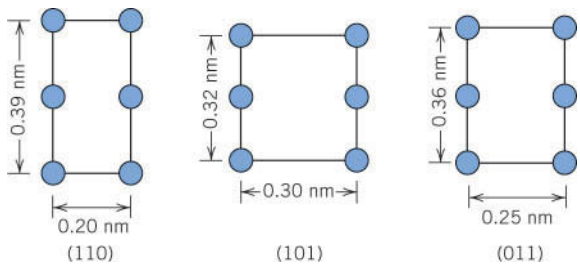
3.53 The accompanying figure shows three different crystallographic planes for a unit cell of a hypothetical metal. The circles represent atoms.



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

(b) What would this crystal structure be called?

3.54 The accompanying figure shows three different crystallographic planes for a unit cell of some hypothetical metal. The circles represent atoms.



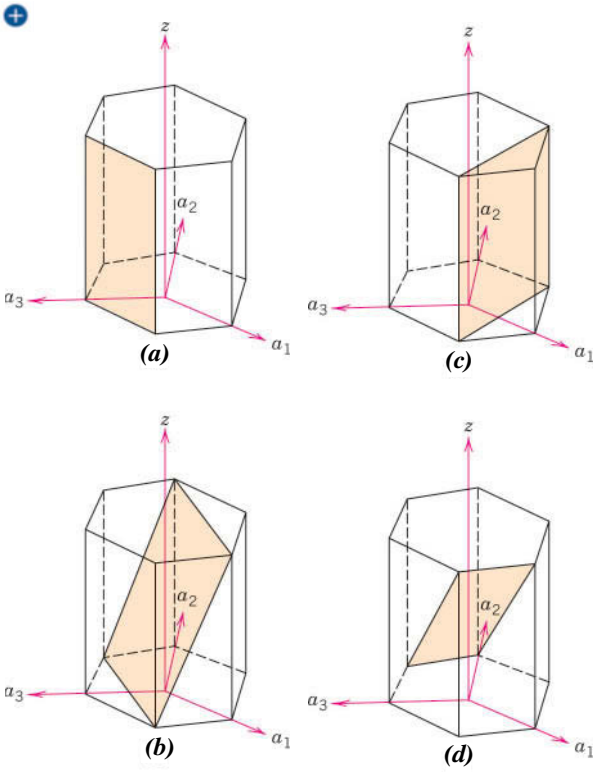
(a) To what crystal system does the unit cell belong?

(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.

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

3.56 Determine the indices for the planes shown in the following hexagonal unit cells:



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

Linear and Planar Densities

3.58 **(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 directions for copper (Cu).

3.59 **(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 directions for iron (Fe).

3.60 **(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 (Al).

3.61 **(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 (Mo).

3.62 **(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 (Ti).

Polycrystalline Materials

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

X-Ray Diffraction: Determination of Crystal Structures

3.64 The interplanar spacing d_{hkl} for planes in a unit cell having orthorhombic geometry is given by

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

where a, b, and c are the lattice parameters.

(a) To what equation does this expression reduce for crystals having cubic symmetry?

(b) For crystals having tetragonal symmetry?

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

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

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

3.68 Determine the expected diffraction angle for the first-order reflection from the (111) set of planes for FCC nickel (Ni) when monochromatic radiation of wavelength 0.1937 nm is used.

3.69 The metal rhodium (Rh) 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 the following:

(a) The interplanar spacing for this set of planes

(b) The atomic radius for a Rh atom

3.70 The metal niobium (Nb) 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 the following:

(a) The interplanar spacing for this set of planes

(b) The atomic radius for the Nb atom

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

3.72 For which set of crystallographic planes will a first-order diffraction peak occur at a diffraction angle of 44.53° for BCC tantalum (Ta) when monochromatic radiation having a wavelength of 0.1937 nm is used?

3.73 Figure 3.26 shows the first five peaks of the x-ray diffraction pattern for tungsten (W), 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) 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.

3.74 The following table lists diffraction angles for the first four peaks (first-order) of the x-ray diffraction pattern for platinum (Pt), which has an FCC crystal structure; monochromatic x-radiation having a wavelength of 0.0711 nm was used.

Plane Indices	*Diffraction Angle (2θ)*
(111)	18.06°
(200)	20.88°
(220)	26.66°
(311)	31.37°

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

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

3.75 The following table lists diffraction angles for the first three peaks (first-order) of the x-ray diffraction pattern for some metal. Monochromatic x-radiation having a wavelength of 0.1397 nm was used.

(a) Determine whether this metal's crystal structure is FCC, BCC, or neither FCC or BCC, and explain the reason for your choice.

(b) If the crystal structure is either BCC or FCC, identify which of the metals in Table 3.1 gives this diffraction pattern. Justify your decision.

Peak Number	*Diffraction Angle (2θ)*
1	34.51°
2	40.06°
3	57.95°

3.76 The following table lists diffraction angles for the first three peaks (first-order) of the x-ray diffraction pattern for some metal. Monochromatic x-radiation having a wavelength of 0.0711 nm was used.

(a) Determine whether this metal's crystal structure is FCC, BCC, or neither FCC or BCC, and explain the reason for your choice.

(b) If the crystal structure is either BCC or FCC, identify which of the metals in Table 3.1 gives this diffraction pattern. Justify your decision.

Peak Number	*Diffraction Angle (2θ)*
1	18.27°
2	25.96°
3	31.92°

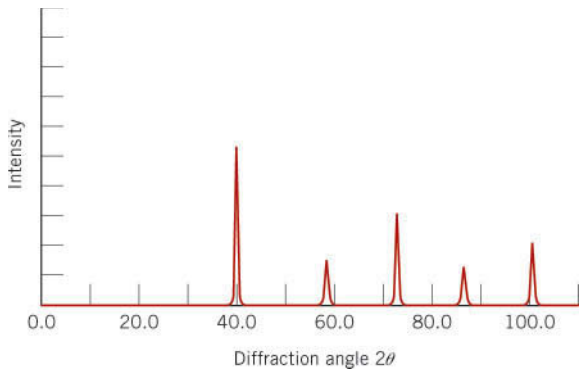


Figure 3.26 Diffraction pattern for powdered tungsten. (Courtesy of Wesley L. Holman.)

Noncrystalline Solids

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

Spreadsheet Problem

3.1SS For an x-ray diffraction pattern (having all peaks plane-indexed) of a metal that has a unit cell of cubic symmetry, generate a spreadsheet that allows the user to input the x-ray wavelength, and then determine, for each plane, the following:

(a) d_{hkl}

(b) The lattice parameter, a

FUNDAMENTALS OF ENGINEERING QUESTIONS AND PROBLEMS

3.1FE A hypothetical metal has the BCC crystal structure, a density of 7.24 g/cm^3, and an atomic weight of 48.9 g/mol. The atomic radius of this metal is

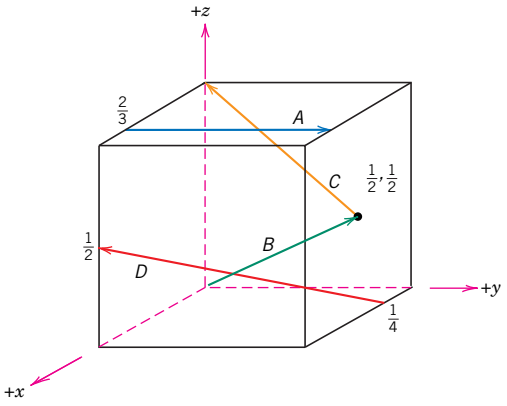
(A) 0.122 nm

(B) 1.22 nm

(C) 0.0997 nm

(D) 0.154 nm

3.2FE In the following unit cell, which vector represents the [121] direction?



3.3FE What are the Miller indices for the plane shown in the following cubic unit cell?

(A) (201)

(B) $(1\infty\frac{1}{2})$

(C) $(10\frac{1}{2})$

(D) (102)