

the structure and properties of amorphous ceramics and polymers is contained in Chapters 13 and 15.

## SUMMARY

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Atoms in crystalline solids are positioned in an orderly and repeated pattern that is in contrast to the random and disordered atomic distribution found in noncrystalline or amorphous materials. Atoms may be represented as solid spheres, and, for crystalline solids, crystal structure is just the spatial arrangement of these spheres. The various crystal structures are specified in terms of parallelepiped unit cells, which are characterized by geometry and atom positions within.

Most common metals exist in at least one of three relatively simple crystal structures: face-centered cubic (FCC), body-centered cubic (BCC), and hexagonal close-packed (HCP). Two features of a crystal structure are coordination number (or number of nearest-neighbor atoms) and atomic packing factor (the fraction of solid sphere volume in the unit cell). Coordination number and atomic packing factor are the same for both FCC and HCP crystal structures, each of which may be generated by the stacking of close-packed planes of atoms.

Crystallographic planes and directions are specified in terms of an indexing scheme. The basis for the determination of each index is a coordinate axis system defined by the unit cell for the particular crystal structure. Directional indices are computed in terms of vector projections on each of the coordinate axes, whereas planar indices are determined from the reciprocals of axial intercepts. For hexagonal unit cells, a four-index scheme for both directions and planes is found to be more convenient.

Crystallographic directional and planar equivalencies are related to atomic linear and planar densities, respectively. The atomic packing (i.e., planar density) of spheres in a crystallographic plane depends on the indices of the plane as well as the crystal structure. For a given crystal structure, planes having identical atomic packing yet different Miller indices belong to the same family.

Single crystals are materials in which the atomic order extends uninterrupted over the entirety of the specimen; under some circumstances, they may have flat faces and regular geometric shapes. The vast majority of crystalline solids, however, are polycrystalline, being composed of many small crystals or grains having different crystallographic orientations.

X-ray diffractometry is used for crystal structure and interplanar spacing determinations. A beam of x-rays directed on a crystalline material may experience diffraction (constructive interference) as a result of its interaction with a series of parallel atomic planes according to Bragg's law. Interplanar spacing is a function of the Miller indices and lattice parameter(s) as well as the crystal structure.

## IMPORTANT TERMS AND CONCEPTS

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Allotropy	Crystal system	Lattice
Amorphous	Crystalline	Lattice parameters
Anisotropy	Diffraction	Miller indices
Atomic packing factor (APF)	Face-centered cubic (FCC)	Noncrystalline
Body-centered cubic (BCC)	Grain	Polycrystalline
Bragg's law	Grain boundary	Polymorphism
Coordination number	Hexagonal close-packed (HCP)	Single crystal
Crystal structure	Isotropic	Unit cell

## REFERENCES

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- Schwartz, L. H. and J. B. Cohen, *Diffraction from Materials*, 2nd edition, Springer-Verlag, New York, 1987.
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## QUESTIONS AND PROBLEMS

- 3.1** What is the difference between atomic structure and crystal structure?
- 3.2** What is the difference between a crystal structure and a crystal system?
- 3.3** If the atomic radius of aluminum is 0.143 nm, calculate the volume of its unit cell in cubic meters.
- 3.4** Show for the body-centered cubic crystal structure that the unit cell edge length  $a$  and the atomic radius  $R$  are related through  $a = 4R/\sqrt{3}$ .
- 3.5** For the HCP crystal structure, show that the ideal  $c/a$  ratio is 1.633.
- 3.6** Show that the atomic packing factor for BCC is 0.68.
- 3.7** Show that the atomic packing factor for HCP is 0.74.
- 3.8** Iron has a BCC crystal structure, an atomic radius of 0.124 nm, and an atomic weight of 55.85 g/mol. Compute and compare its density with the experimental value found inside the front cover.
- 3.9** Calculate the radius of an iridium atom given that Ir has an FCC crystal structure, a density of 22.4 g/cm<sup>3</sup>, and an atomic weight of 192.2 g/mol.
- 3.10** Calculate the radius of a vanadium atom, given that V has a BCC crystal structure, a density of 5.96 g/cm<sup>3</sup>, and an atomic weight of 50.9 g/mol.
- 3.11** Some hypothetical metal has the simple cubic crystal structure shown in Figure 3.22. If its atomic weight is 70.4 g/mol and the atomic radius is 0.126 nm, compute its density.
- 3.12** Zirconium has an HCP crystal structure and a density of 6.51 g/cm<sup>3</sup>.
- (a) What is the volume of its unit cell in cubic meters?
- (b) If the  $c/a$  ratio is 1.593, compute the values of  $c$  and  $a$ .

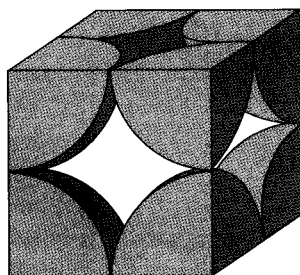


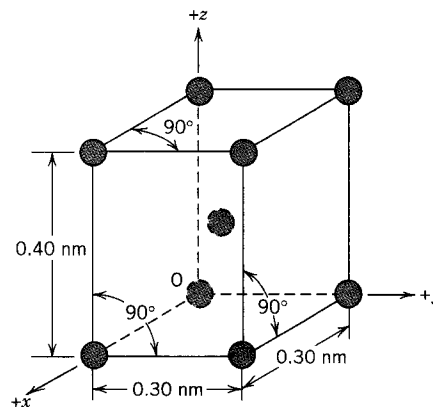
FIGURE 3.22 Hard-sphere unit cell representation of the simple cubic crystal structure.

- 3.13** Using atomic weight, crystal structure, and atomic radius data tabulated inside the front cover, compute the theoretical densities of lead, chromium, copper, and cobalt, and then compare these values with the measured densities listed in this same table. The  $c/a$  ratio for cobalt is 1.623.
- 3.14** Rhodium has an atomic radius of 0.1345 nm (1.345 Å) and a density of 12.41 g/cm<sup>3</sup>. Determine whether it has an FCC or BCC crystal structure.
- 3.15** 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 3.22.

Alloy	Atomic Weight (g/mol)	Density (g/cm <sup>3</sup> )	Atomic Radius (nm)
A	77.4	8.22	0.125
B	107.6	13.42	0.133
C	127.3	9.23	0.142

- 3.16** The unit cell for tin has tetragonal symmetry, with  $a$  and  $b$  lattice parameters of 0.583 and 0.318 nm, respectively. If its density, atomic weight, and atomic radius are 7.30 g/cm<sup>3</sup>, 118.69 g/mol, and 0.151 nm, respectively, compute the atomic packing factor.
- 3.17** Iodine has an orthorhombic unit cell for which the  $a$ ,  $b$ , and  $c$  lattice parameters are 0.479, 0.725, and 0.978 nm, respectively.
- (a) If the atomic packing factor and atomic radius are 0.547 and 0.177 nm, respectively, determine the number of atoms in each unit cell.
- (b) The atomic weight of iodine is 126.91 g/mol; compute its density.
- 3.18** Titanium has an HCP unit cell for which the ratio of the lattice parameters  $c/a$  is 1.58. If the radius of the Ti atom is 0.1445 nm, (a) determine the unit cell volume, and (b) calculate the density of Ti and compare it with the literature value.

- 3.19** Zinc has an HCP crystal structure, a  $c/a$  ratio of 1.856, and a density of 7.13 g/cm<sup>3</sup>. Calculate the atomic radius for Zn.
- 3.20** Rhenium has an HCP crystal structure, an atomic radius of 0.137 nm, and a  $c/a$  ratio of 1.615. Compute the volume of the unit cell for Re.
- 3.21** This 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.
- 3.22** Using the Molecule Definition File (MDF) on the CD-ROM that accompanies this book, generate a three-dimensional unit cell for the intermetallic compound AuCu<sub>3</sub> 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.
- 3.23** Using the Molecule Definition File (MDF) on the CD-ROM that accompanies this book, generate a three-dimensional unit cell for the intermetallic compound AuCu given the following: 1) the unit cell is tetragonal with  $a = 0.289$  nm and  $c = 0.367$  nm (see Table 3.2), 2) gold atoms are situated at all unit cell corners, and 3) a copper atom is positioned at the center of the unit cell.

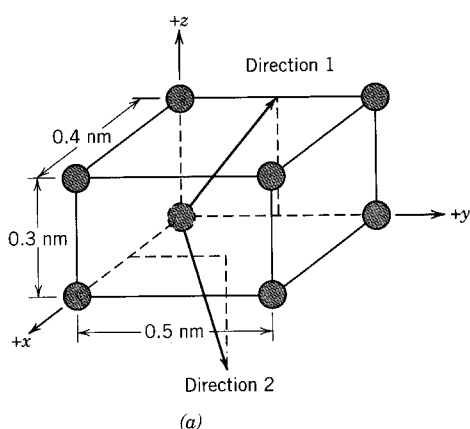
**3.24** Sketch a unit cell for the body-centered orthorhombic crystal structure.

**3.25** Draw an orthorhombic unit cell, and within that cell a  $[1\bar{2}\bar{1}]$  direction and a  $(210)$  plane.

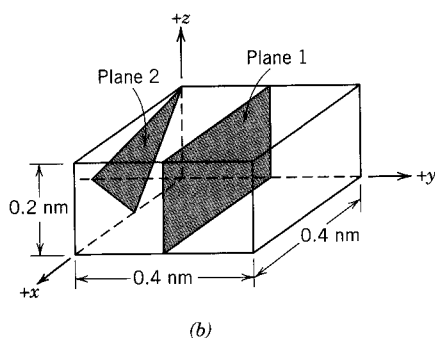
**3.26** Sketch a monoclinic unit cell, and within that cell a  $[0\bar{1}1]$  direction and a  $(002)$  plane.

**3.27** Here are unit cells for two hypothetical metals:

(a) What are the indices for the directions indicated by the two vectors in sketch (a)?



(b) What are the indices for the two planes drawn in sketch (b)?

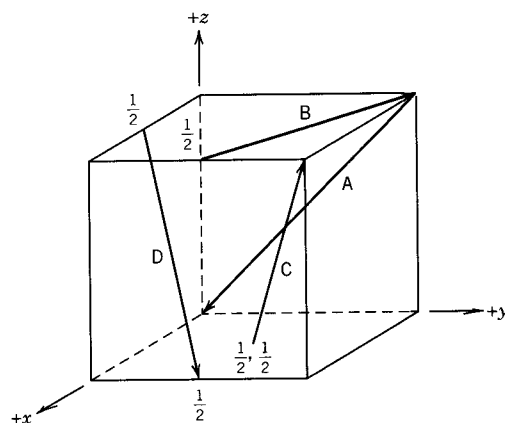


**3.28** Within a cubic unit cell, sketch the following directions:

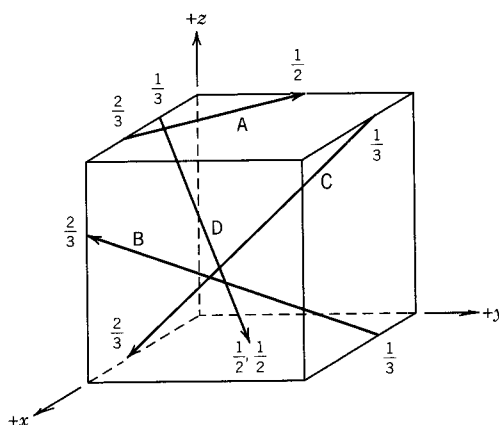


- (a)  $[\bar{1}10]$ ; (e)  $[\bar{1}\bar{1}1]$   
 (b)  $[\bar{1}\bar{2}1]$ ; (f)  $[\bar{1}22]$   
 (c)  $[0\bar{1}2]$ ; (g)  $[1\bar{2}\bar{3}]$   
 (d)  $[1\bar{3}\bar{3}]$ ; (h)  $[\bar{1}0\bar{3}]$ .

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



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



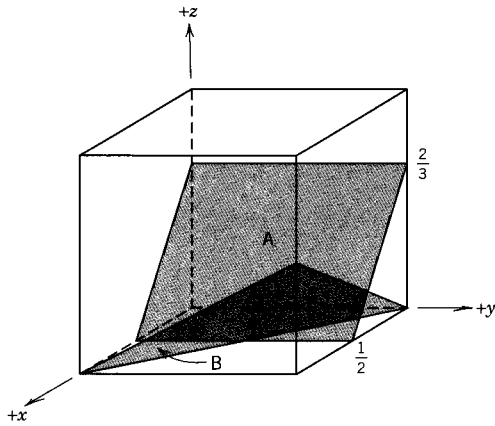
**3.31** For tetragonal crystals, cite the indices of directions that are equivalent to each of the following directions:

- (a)  $[101]$ ;  
 (b)  $[110]$ ;  
 (c)  $[010]$ .

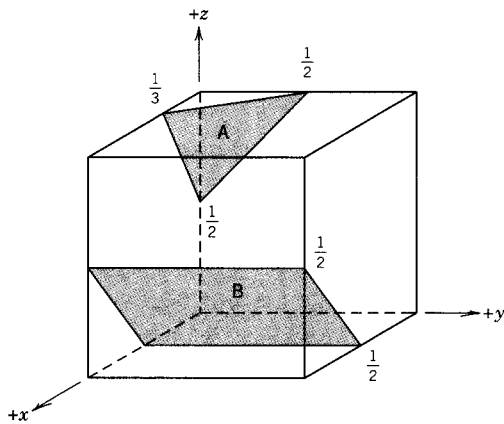
**3.32 (a)** Convert the  $[100]$  and  $[111]$  directions into the four-index Miller-Bravais scheme for hexagonal unit cells.

**(b)** Make the same conversion for the  $(010)$  and  $(101)$  planes.

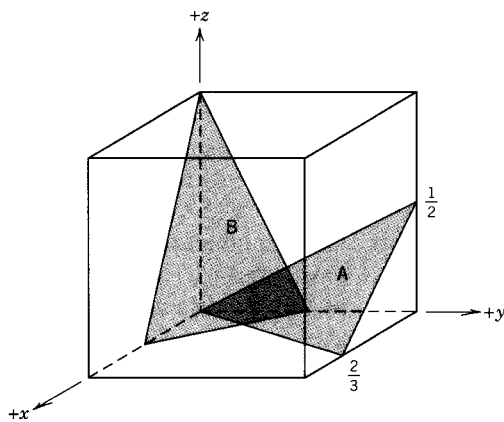
**3.33** Determine the Miller indices for the planes shown in the following unit cell:



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



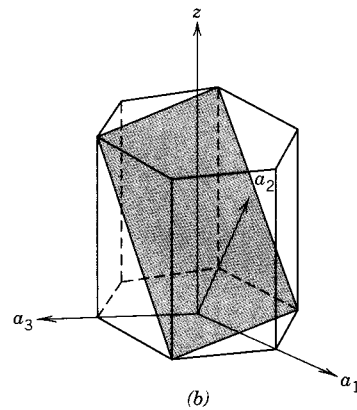
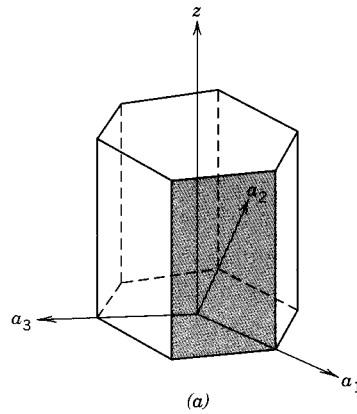
**3.35** Determine the Miller indices for the planes shown in the following unit cell:



**3.36** Sketch the  $(\bar{1}\bar{1}01)$  and  $(1\bar{1}20)$  planes in a hexagonal unit cell.



**3.37** Determine the indices for the planes shown in the hexagonal unit cells shown below.



**3.38** Sketch within a cubic unit cell the following planes:



- (a)  $(0\bar{1}\bar{1})$ ;      (e)  $(\bar{1}\bar{1}\bar{1})$ ;
- (b)  $(11\bar{2})$ ;      (f)  $(1\bar{2}\bar{2})$ ;
- (c)  $(10\bar{2})$ ;      (g)  $(\bar{1}\bar{2}\bar{3})$ ;
- (d)  $(\bar{1}\bar{3}1)$ ;      (h)  $(0\bar{1}\bar{3})$ .

**3.39** 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 3.9b and 3.10b).

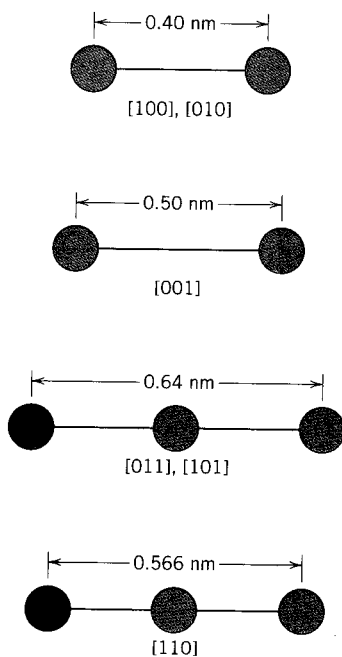
**3.40** Consider the reduced-sphere unit cell shown in Problem 3.21, having an origin of the coordinate system positioned at the atom labeled

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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 ( $\bar{1}\bar{1}$ 0).
- (c) (111), ( $\bar{1}\bar{1}\bar{1}$ ), (11 $\bar{1}$ ), and ( $\bar{1}\bar{1}\bar{1}$ ).

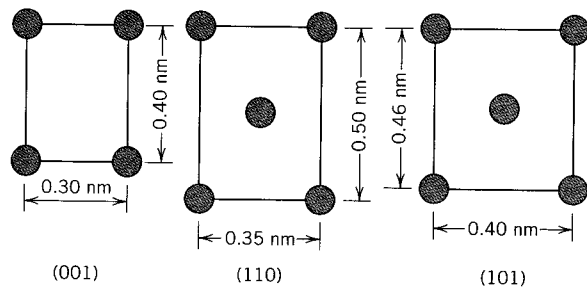
- 3.41** Cite the indices of the direction that results from the intersection of each of the following pair of planes within a cubic crystal: (a) (110) and (111) planes; (b) (110) and ( $\bar{1}\bar{1}$ 0) planes; and (c) (10 $\bar{1}$ ) and (001) planes.
- 3.42** Compute and compare the linear densities of the [100], [110], and [111] directions for FCC.
- 3.43** Compute and compare the linear densities of the [110] and [111] directions for BCC.
- 3.44** Calculate and compare the planar densities of the (100) and (111) planes for FCC.
- 3.45** Calculate and compare the planar densities of the (100) and (110) planes for BCC.
- 3.46** Calculate the planar density of the (0001) plane for HCP.
- 3.47** Here are shown the atomic packing schemes for several different crystallographic directions for some hypothetical metal. For each direction the circles represent only those atoms contained within a unit cell, which circles are reduced from their actual size.



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

(b) What would this crystal structure be called?

- 3.48** 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 8.95 g/cm<sup>3</sup>, determine its atomic weight.

- 3.49** Explain why the properties of polycrystalline materials are most often isotropic.
- 3.50** Using the data for molybdenum in Table 3.1, compute the interplanar spacing for the (111) set of planes.
- 3.51** Determine the expected diffraction angle for the first-order reflection from the (113) set of planes for FCC platinum when monochromatic radiation of wavelength 0.1542 nm is used.
- 3.52** Using the data for aluminum in Table 3.1, compute the interplanar spacings for the (110) and (221) sets of planes.
- 3.53** The metal iridium has an FCC crystal structure. If the angle of diffraction for the (220) set of planes occurs at 69.22° (first-order reflection) when monochromatic x-radiation having a wavelength of 0.1542 nm is used, compute (a) the interplanar spacing for this set of planes, and (b) the atomic radius for an iridium atom.
- 3.54** The metal rubidium has a BCC crystal structure. If the angle of diffraction for the (321)

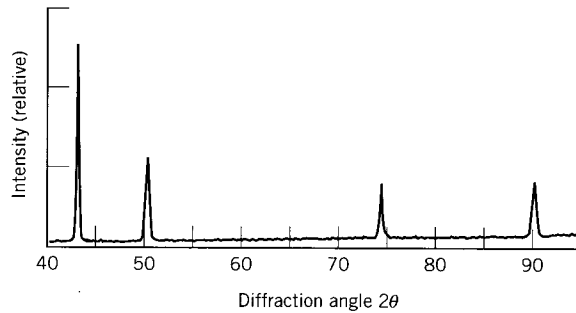


FIGURE 3.23 Diffraction pattern for polycrystalline copper.

set of planes occurs at  $27.00^\circ$  (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 the rubidium atom.

- 3.55** For which set of crystallographic planes will a first-order diffraction peak occur at a diffraction angle of  $46.21^\circ$  for BCC iron when monochromatic radiation having a wavelength of 0.0711 nm is used?
- 3.56** Figure 3.20 shows an x-ray diffraction pattern for  $\alpha$ -iron 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 Fe for each of the peaks.
- 3.57** The diffraction peaks shown in Figure 3.20 are indexed according to the reflection rules for BCC (i.e., the sum  $h + k + l$  must be

even). Cite the  $h$ ,  $k$ , and  $l$  indices for the first four diffraction peaks for FCC crystals consistent with  $h$ ,  $k$ , and  $l$  all being either odd or even.

- 3.58** Figure 3.23 shows the first four peaks of the x-ray diffraction pattern for copper, which has an FCC 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 Cu and compare these with the value presented in Table 3.1.
- 3.59** Would you expect a material in which the atomic bonding is predominantly ionic in nature to be more or less likely to form a non-crystalline solid upon solidification than a covalent material? Why? (See Section 2.6.)