CHAPTER 3

THE STRUCTURE OF CRYSTALLINE SOLIDS

PROBLEM SOLUTIONS

Fundamental Concepts

3.1 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.

Unit Cells

Metallic Crystal Structures

3.2 For this problem, we are asked to calculate the volume of a unit cell of lead. Lead has an FCC crystal structure (Table 3.1). The FCC unit cell volume may be computed from Equation 3.4 as

$$V_C = 16R^3\sqrt{2} = (16)(0.175 \times 10^{-9}\ \text{m})^3(\sqrt{2}) = 1.213 \times 10^{-28}\ \text{m}^3$$

Density Computations

3.7 This problem calls for a computation of the density of molybdenum. According to Equation 3.5

$$\rho = \frac{nA_{\text{Mo}}}{V_C N_{\text{A}}}$$

For BCC, n = 2 atoms/unit cell, and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3$$

Thus,

$$\rho = \frac{nA_{\text{Mo}}}{\left(\frac{4R}{\sqrt{3}}\right)^3 N_{\text{A}}}$$

$$= \frac{\text{(2 atoms/unit cell)(95.94 g/mol)}}{\left[(4)\left(0.1363 \times 10^{-7}\ \text{cm}\right)^3/\sqrt{3}\right]^3/\text{(unit cell)}\left(6.023 \times 10^{23}\ \text{atoms/mol}\right)}$$

$$= 10.21\ \text{g/cm}^3$$

The value given inside the front cover is 10.22 g/cm^3.

3.9 This problem asks for us to calculate the radius of a tantalum atom. For BCC, n = 2 atoms/unit cell, and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64R^3}{3\sqrt{3}}$$

Since, from Equation 3.5

$$\rho = \frac{nA_{\mathrm{Ta}}}{V_C N_\mathrm{A}}$$

$$= \frac{nA_{\mathrm{Ta}}}{\left(\frac{64R^3}{3\sqrt{3}}\right) N_\mathrm{A}}$$

and solving for R the previous equation

$$R = \left(\frac{3\sqrt{3}nA_{\mathrm{Ta}}}{64\rho N_\mathrm{A}}\right)^{1/3}$$

$$= \left[\frac{(3\sqrt{3})(2 \text{ atoms/unit cell})(180.9 \text{ g/mol})}{(64)(16.6 \text{ g/cm}^3)(6.023 \times 10^{23} \text{ atoms/mol})}\right]^{1/3}$$

$$= 1.43 \times 10^{-8} \text{ cm} = 0.143 \text{ nm}$$

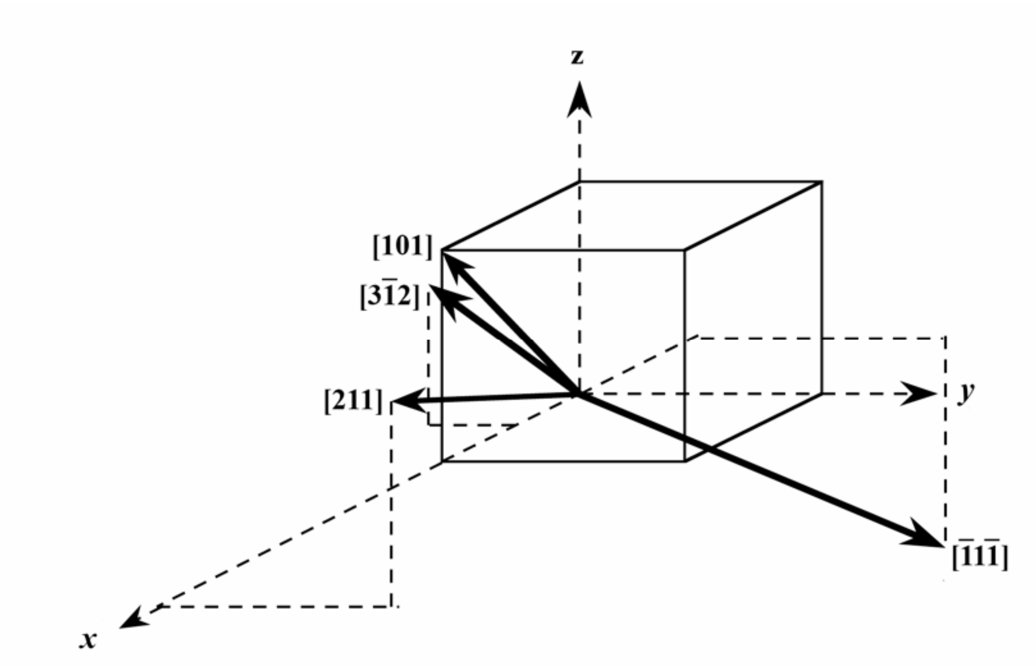
3.10 For the simple cubic crystal structure, the value of n in Equation 3.5 is unity since there is only a single atom associated with each unit cell. Furthermore, for the unit cell edge length, a = 2R (Figure 3.23). Therefore, employment of Equation 3.5 yields

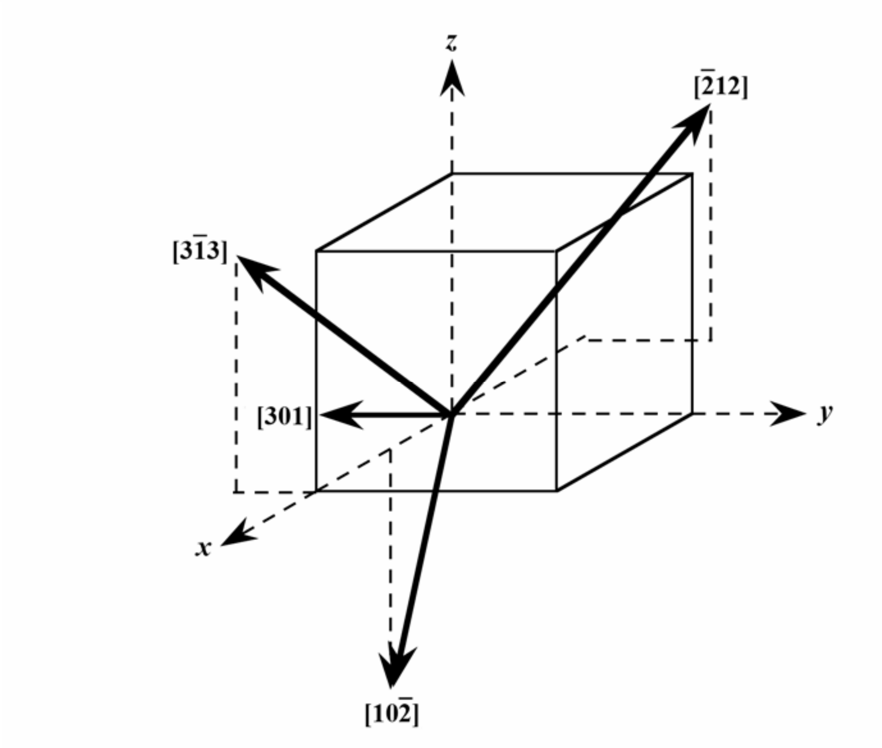
$$\rho = \frac{nA}{V_C N_A} = \frac{nA}{(2R)^3 N_A}$$

$$= \frac{\text{(1 atom/unit cell)(74.5 g/mol)}}{\left\{\left[(2)\left(1.45 \times 10^{-8}\ \text{cm}\right)\right]^3 \text{/(unit cell)}\right\}\left(6.023 \times 10^{23}\ \text{atoms/mol}\right)}$$

$$5.07\ \text{g/cm}^3$$

3.30 The directions asked for are indicated in the cubic unit cells shown below.





3.31 Direction A is a $[\bar{1}10]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	$-a$	b	$0c$
Projections in terms of *a*, *b*, and *c*	–1	1	0
Reduction to integers		not necessary	
Enclosure		$[\bar{1}10]$	

Direction B is a [121] direction, which determination is summarized as follows. The vector passes through the origin of the coordinate system and thus no translation is necessary. Therefore,

	x	y	z
Projections	$\frac{a}{2}$	b	$\frac{c}{2}$
Projections in terms of *a*, *b*, and *c*	$\frac{1}{2}$	1	$\frac{1}{2}$
Reduction to integers	1	2	1
Enclosure		[121]	

Direction C is a $[0\bar{1}\bar{2}]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	$0a$	$-\frac{b}{2}$	$-c$
Projections in terms of *a*, *b*, and *c*	0	$-\frac{1}{2}$	–1
Reduction to integers	0	–1	–2
Enclosure		$[0\bar{1}\bar{2}]$	

Direction D is a $[1\bar{2}1]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	$\frac{a}{2}$	$-b$	$\frac{c}{2}$
Projections in terms of *a*, *b*, and *c*	$\frac{1}{2}$	–1	$\frac{1}{2}$
Reduction to integers	1	–2	1
Enclosure		$[1\bar{2}1]$	

3.38 This problem calls for specification of the indices for the two planes that are drawn in the sketch.

Plane 1 is a (211) plane. The determination of its indices is summarized below.

	x	y	z
Intercepts	*a*/2	*b*	*c*
Intercepts in terms of *a*, *b*, and *c*	1/2	1	1
Reciprocals of intercepts	2	1	1
Enclosure		(211)	

Plane 2 is a $(0\overline{2}0)$ plane, as summarized below.

	x	y	z
Intercepts	∞*a*	-*b*/2	∞*c*
Intercepts in terms of *a*, *b*, and *c*	∞	-1/2	∞
Reciprocals of intercepts	0	-2	0
Enclosure		$(0\overline{2}0)$	

3.42 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 vertically along the *z* axis; thus, this is a $(21\overline{1})$ plane, as summarized below.

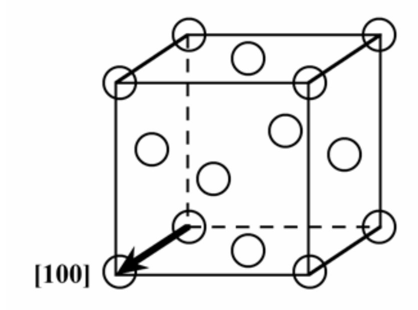
	$\underline{x}$	$\underline{y}$	$\underline{z}$
Intercepts	$\frac{a}{2}$	b	$-c$
Intercepts in terms of *a*, *b*, and *c*	$\frac{1}{2}$	1	– 1
Reciprocals of intercepts	2	1	– 1
Reduction		not necessary	
Enclosure		$(21\overline{1})$	

For plane B, since the plane passes through the origin of the coordinate system as shown, we will move the origin one unit cell distance vertically along the *z* axis; this is a $(02\overline{1})$ plane, as summarized below.

	$\underline{x}$	$\underline{y}$	$\underline{z}$
Intercepts	$\infty\, a$	$\frac{b}{2}$	$-c$
Intercepts in terms of *a*, *b*, and *c*	∞	$\frac{1}{2}$	– 1
Reciprocals of intercepts	0	2	– 1
Reduction		not necessary	
Enclosure		$(02\overline{1})$	

Linear and Planar Densities

3.51 (a) In the figure below is shown a [100] direction within an FCC unit cell.

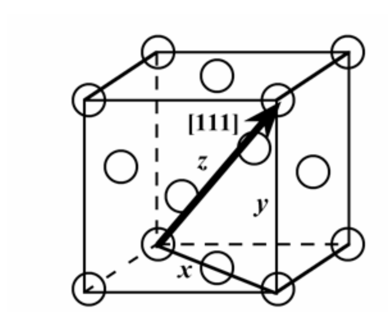


For this [100] direction there is one atom at each of the two unit cell corners, and, thus, there is the equivalent of 1 atom that is centered on the direction vector. The length of this direction vector is just the unit cell edge length, $2R\sqrt{2}$ (Equation 3.1). Therefore, the expression for the linear density of this plane is

$$\mathrm{LD}_{100} = \frac{\text{number of atoms centered on [100] direction vector}}{\text{length of [100] direction vector}}$$

$$= \frac{1 \text{ atom}}{2R\sqrt{2}} = \frac{1}{2R\sqrt{2}}$$

An FCC unit cell within which is drawn a [111] direction is shown below.



For this [111] direction, the vector shown passes through only the centers of the single atom at each of its ends, and, thus, there is the equivalence of 1 atom that is centered on the direction vector. The length of this direction vector is denoted by z in this figure, which is equal to

$$z = \sqrt{x^2 + y^2}$$