

12.23 We are asked in this problem to compute the atomic packing factor for the diamond cubic crystal structure, given that the angle between adjacent bonds is 109.5° . The first thing that we must do is to determine the unit cell volume V_C in terms of the atomic radius r . From Problem 12.15 the following relationship was developed

$$a = 4y \sin \theta$$

in which $y = 2r$ and $\theta = 35.25^\circ$. Furthermore, since the unit cell is cubic, $V_C = a^3$; therefore

$$V_C = (4y \sin \theta)^3 = [(4)(2r)(\sin 35.25^\circ)]^3 = 98.43 r^3$$

Now, it is necessary to determine the sphere volume in the unit cell, V_S , in terms of r . For this unit cell (Figure 12.15) there are 4 interior atoms, 6 face atoms, and 8 corner atoms. The entirety of the interior atoms, one-half of each face atom, and one-eighth of each corner atom belong to the unit cell. Therefore, there are 8 equivalent atoms per unit cell; hence

$$V_S = (8) \left(\frac{4}{3} \pi r^3 \right) = 33.51 r^3$$

Finally, the atomic packing factor is just

$$\text{APF} = \frac{V_S}{V_C} = \frac{33.51 r^3}{98.43 r^3} = 0.340$$