

Chapter 1 Homework Solutions

1. For a face centered cubic lattice of identical atoms, with a lattice constant of 4.5 \AA , find the following:

- a. Maximum packing fraction.

The face centered cube has 4 equivalent atoms ($1/8^{\text{th}}$ times 8 corners + $1/2$ each times 6 faces). Therefore the packing factor is the volume of 4 atoms divided into the volume of the unit cell. The unit cell volume is simply a^3 or 91.125 \AA^3 .

Using the formula for the volume of a sphere, $V = \frac{4}{3}\pi r^3$, and the atomic radius r of 1.59 \AA (from part b. of this problem), we calculate the volume of the 4 atoms to be

$$V = (4) \frac{4}{3} \pi (1.59 \text{ \AA})^3 = 67.35 \text{ \AA}^3.$$

Thus the packing factor is $P.F. = \frac{67.35}{91.125} \text{ \AA}^3 = 74\%$

- b. Radius of atoms treated as hard spheres.

The hard sphere model would line up 3 atoms along the face diagonal of the cube, with the end two extending only one radius into the cube's face. Thus the face diagonal would equal 4 atomic radii in length (one each from the corner atoms, and two radii from the center face atom). Applying Pythagoras' theorem; $a^2 + b^2 = c^2$; $a^2 + a^2 = (4r)^2$ or $4r = \sqrt{2a^2}$ thus $r = \frac{\sqrt{2}}{4}a$. We find that r is 1.59 \AA .

2. A Si crystal is to be grown by the Czochralski method, and is desired to contain 1.7×10^{16} Boron atoms per cm^3 . Presuming a k_d of 0.28, how many grams of Boron must be added to the 10 kg Si melt to obtain this Boron concentration? [Hint: Example 1-4, p 17]

If only 28% of the Boron moves from the liquid to the solid, and we want 1.7×10^{16} Boron atoms per cm^3 in the solid, we must start with $1.7 \times 10^{16} / 0.28$ atoms per cm^3 in the liquid melt. So our melt must contain 6.07×10^{16} Boron atoms per cm^3 .

Using the density of Si of 2.33 g/cm^3 , we calculate that 10 kg of Si will have a volume of 4992 cm^3 . That much Si will require $(4992)(6.07 \times 10^{16}) = 2.6 \times 10^{20}$ Boron atoms.

2.6×10^{20} Boron atoms weigh $(2.6 \times 10^{20} \text{ Boron atoms}) \times (10.8 \text{ g/mole of Boron}) / 6.0 \times 10^{23} \text{ atoms/mole} = 4.664 \times 10^{-3} \text{ grams}$ or 4.664 milligrams of Boron

3. Problem 1.16, p27.

The sketch should look something like that in figure 1-8a. The assignment was just to force you to think about it.