Chapter 1 Solutions

Prob. 1.1

Which semiconductor in Table 1-1 has the largest E_g? the smallest? What is the corresponding λ? How is the column III component related to E_g?

largest E_g : ZnS, 3.6 eV

$$\lambda = \frac{1.24}{3.6} = 0.344\mu m$$

smallest E_g : InSb, 0.18 eV

$$\lambda = \frac{1.24}{0.18} = 6.89\mu m$$

Al compounds E_g > corresponding Ga compounds E_g > the corresponding In compounds E_g

Prob. 1.2

For a bcc lattice of identical atoms with a lattice constant of 5 Å, calculate the maximum packing fraction and the radius of the atoms treated as hard spheres with the nearest neighbors touching.

Each corner atom in a cubic unit cell is shared with seven neighboring cells; thus, each unit cell contains one-eighth of a sphere at each of the eight corners for a total of one atom. The bcc cell contains one atom in the center of the cube. Thus, we have

Nearest atoms are at a separation $\frac{1}{2} \times \sqrt{5^2 + 5^2 + 5^2} = 4.330$ Å

$$\text{Radius of each atom} = \frac{1}{2} \times 4.330 \text{ Å} = 2.165 \text{ Å}$$

$$\text{Volume of each atom} = \frac{4}{3}\pi(2.165)^3 = 42.5 \text{ Å}^3$$

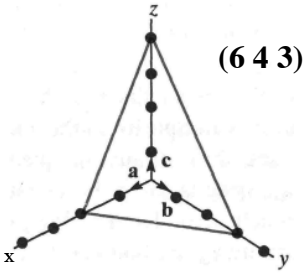
Number of atoms per cube $= 1 + 8 \times \frac{1}{8} = 2$

Packing fraction $= \frac{42.5 \times 2}{(5)^3} = 68\%.$

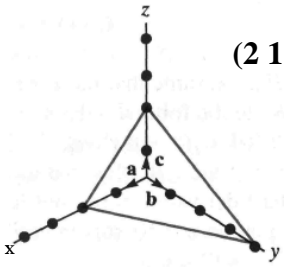
Therefore, if the atoms in a bcc lattice are packed as densely as possible, with no distance between the outer edges of nearest neighbors, 68% of the volume is filled. This is a relatively high percentage compared with some other lattice structures.

Prob. 1.3

Label planes.



(6 4 3)



(2 1 2)

x	y	z
2	3	4
1/2	1/3	1/4
6	4	3

x	y	z
2	4	2
1/2	1/4	1/2
2	1	2

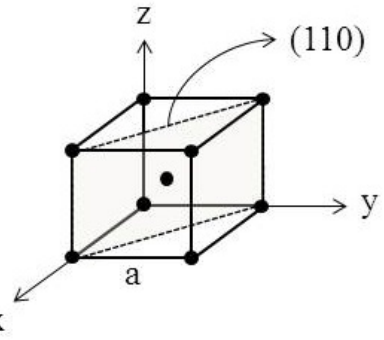
Prob.1.4

Sketch a *body centered cubic* unit cell with a monoatomic basis. If the atomic density is $1.6\text{x}10^{22}$ cm^{-3}, calculate the lattice constant. What is the atomic density per unit area on the (110) plane? What is the radius of each atom? What are interstitials and vacancies?

$$\#\text{ of atoms in unit cell } a^3 = 8\times\frac{1}{8}+1=2$$

$$\frac{2}{a^3}=1.6\times10^{22}\text{cm}^{-3}$$

$$a=\left(\frac{1}{8}\right)^{\frac{1}{3}}\times10^{-7}\text{cm}=5\approx$$



$$\text{Area of (110) plane} = \left(a\sqrt{2}\right)a=\sqrt{2}\left(25\right)\approx\ ^2$$

$$\#\text{ of atoms} = 1+4\times\frac{1}{4}=2 \Rightarrow \text{Density} = \frac{2}{\sqrt{2}\left(25\right)}\text{Å}^{-2}$$

$$=\frac{0.707\times2\times10^{16}}{25}\ \#/\text{cm}^2=5.6\times10^{14}\ \text{cm}^{-2}$$

$$\text{Nearest neighbor atoms along body diagonal} = \frac{\sqrt{3}a}{2}$$

$$\text{Radius} = \frac{\sqrt{3}}{4}a = 2.17\text{Å}$$

Vacancies are missing atoms. Interstitials are extra atoms in between atoms (voids).

Prob. 1.5

Calculate densities of Si and GaAs.

The atomic weights of Si, Ga, and As are 28.1, 69.7, and 74.9, respectively.

Si: $a = 5.43 \cdot 10^{-8}$ cm, 8 atoms/cell

$$\frac{8 \text{ atoms}}{a^3} = \frac{8}{\left(5.43 \cdot 10^{-8} \text{cm}\right)^3} = 5 \cdot 10^{22} \frac{1}{\text{cm}^3}$$

$$\text{density} = \frac{5 \cdot 10^{22} \frac{1}{\text{cm}^3} \cdot 28.1 \frac{\text{g}}{\text{mol}}}{6.02 \cdot 10^{23} \frac{1}{\text{mol}}} = 2.33 \frac{\text{g}}{\text{cm}^3}$$

GaAs: $a = 5.65 \cdot 10^{-8}$ cm, 4 each Ga, As atoms/cell

$$\frac{4}{a^3} = \frac{4}{\left(5.65 \cdot 10^{-8} \text{cm}\right)^3} = 2.22 \cdot 10^{22} \frac{1}{\text{cm}^3}$$

$$\text{density} = \frac{2.22 \cdot 10^{22} \frac{1}{\text{cm}^3} \cdot \left(69.7 + 74.9\right) \frac{\text{g}}{\text{mol}}}{6.02 \cdot 10^{23} \frac{1}{\text{mol}}} = 5.33 \frac{\text{g}}{\text{cm}^3}$$

Prob. 1.6

For InSb, find lattice constant, primitive cell volume, (110) atomic density.

$$\frac{\sqrt{3}a}{4} = 1.44\text{Å} + 1.36\text{Å} = 2.8\text{Å}$$

$a = 6.47\text{Å}$

FCC unit cell has 4 lattice points $\therefore$ volume of primitive cell $= \frac{a^3}{4} = 67.7\text{Å}^3$

area of (110) plane $= \sqrt{2}a^2$

density of In atoms $= \frac{4 \cdot \frac{1}{4} + 2 \cdot \frac{1}{2}}{\sqrt{2}\,a^2} = \frac{\sqrt{2}}{a^2} = 3.37 \cdot 10^{14} \frac{1}{\text{cm}^2}$

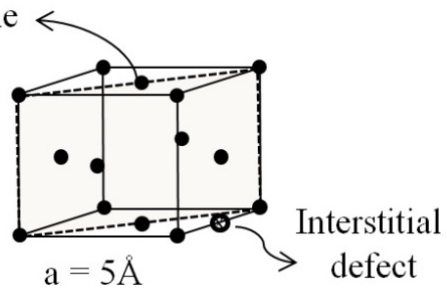
same number of Sb atoms $= 3.37 \cdot 10^{14} \frac{1}{\text{cm}^2}$

Prob. 1.7

Sketch an FCC lattice unit cell (lattice constant = 5Å) with a monoatomic basis, and calculate the atomic density per unit area on (110) planes. What is the atomic density per unit volume? Indicate an interstitial defect in this cell?

$$\text{Area of (110) plane} = a\left(a\sqrt{2}\right)$$

$$= \left(5\left(5\sqrt{2}\right)\text{Å}\right)^2$$



$$\text{Number of atoms} = 4\times\frac{1}{4} + 2\times\frac{1}{2} = 2$$

$$\text{Areal density} = \frac{2}{25\sqrt{2}}\ \text{atoms/Å}^2$$

$$\left(1\text{Å} = 10^{-8}\text{cm}\right)$$

$$= 0.057\times10^{16}\ \text{atoms/cm}^2$$

$$= 5.7\times10^{14}\ \text{atoms/cm}^2$$

$$\text{Volume of unit cells} = a^3 = \left(125\right)\text{Å}^3 = 1.25\times10^{-22}\ \text{cm}^3$$

$$\text{Number of atoms/unit cell} = 8\times\frac{1}{8} + 6\times\frac{1}{2} = 4$$

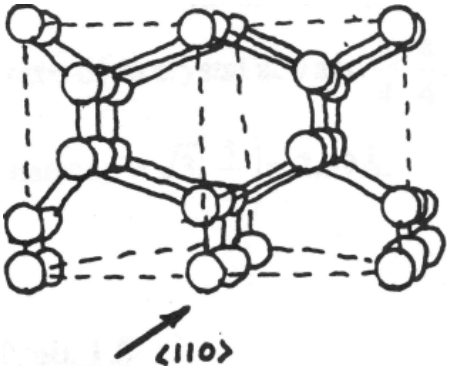
$$\text{Volume density} = \frac{4}{1.25\times10^{-22}}\ \text{atoms/cm}^3$$

$$= 3.2\times10^{22}\ \text{atoms/cm}^3$$

An interstitial defect is marked on the FCC sketch above.

Prob. 1.8

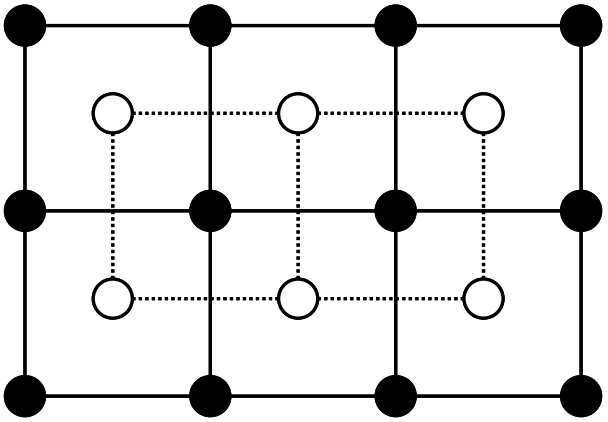
Draw <110> direction of diamond lattice.

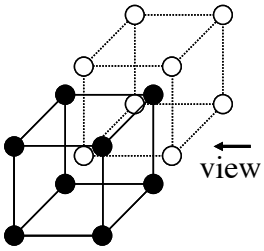


This view is tilted slightly from (110) to show the alignment of atoms. The open channels are hexagonal along this direction.

Prob. 1.9

Show bcc lattice as interpenetrating sc lattices.

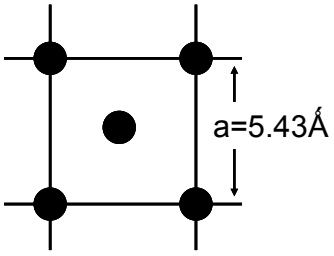




The shaded points are one sc lattice. The open points are the interpenetrating sc lattice located a/2 behind the plane of the front shaded points.

Prob. 1.10

(a) Find number of Si atoms/cm^2 on (100) surface.

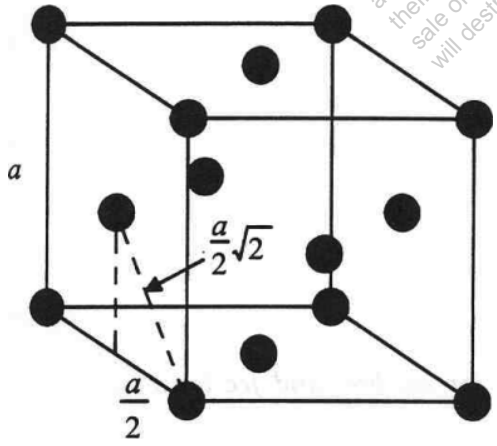


fcc lattice with a $= 5.43\text{Å}$

number atoms per (100) surface $= 4 \cdot \frac{1}{4} + 1 = 2$ atoms

atoms per (100) surface area $= \dfrac{2}{\left(5.43\text{Å}\right)^2} = 6.78 \cdot 10^{14} \frac{1}{\text{cm}^2}$

(b) Find the nearest neighbor distance in InP.



fcc lattice with a $= 5.87\text{Å}$

nearest neighbor distance $= \dfrac{a}{2} \cdot \sqrt{2} = \dfrac{5.87\text{Å}}{2} \cdot \sqrt{2} = 4.15\text{Å}$

Prob. 1.11

Find NaCl density.
Na^+: atomic weight 23g/mol, radius 1Å
Cl^-: atomic weight 35.5g/mol, radius 1.8Å

unit cell with a $= 2.8\text{Å}$ by hard sphere approximation

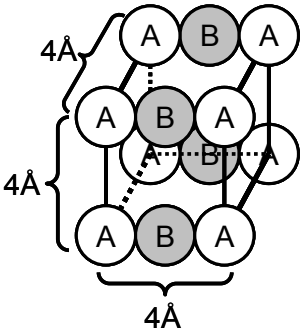
½ Na and ½ Cl atoms per unit cell $= \frac{\frac{1}{2}\frac{\text{atoms}}{\text{cell}}\cdot 23\frac{\text{g}}{\text{mol}} + \frac{1}{2}\frac{\text{atoms}}{\text{cell}}\cdot 35.5\frac{\text{g}}{\text{mol}}}{6.02\cdot 10^{23}\frac{\text{atoms}}{\text{mol}}} = 4.86\cdot 10^{-23}\frac{\text{g}}{\text{cell}}$

density $= \frac{4.86\cdot 10^{-23}\frac{\text{g}}{\text{cell}}}{(2.8\cdot 10^{-8}\text{cm})^3\frac{1}{\text{cell}}} = 2.2\frac{\text{g}}{\text{cm}^3}$

The hard sphere approximation is comparable with the measured $2.17\frac{\text{g}}{\text{cm}^3}$ density.

Prob. 1.12

Find packing fraction, B atoms per unit volume, and A atoms per unit area.



Note: The atoms are the same size and touch each other by the hard sphere approximation.

radii of A and B atoms are then 1Å

number of A atoms per unit cell $= 8\cdot\frac{1}{8} = 1$

number of B atoms per unit cell $= 1$

volume of atoms per unit cell $= 1\cdot\frac{4\pi}{3}\cdot(1\text{Å})^3 + 1\cdot\frac{4\pi}{3}\cdot(1\text{Å})^3 = \frac{8\pi}{3}\text{Å}^3$

volume of unit cell $= (4\text{Å})^3 = 64\text{Å}^3$

packing fraction $= \frac{\frac{8\pi}{3}\text{Å}^3}{64\text{Å}^3} = \frac{\pi}{24} = 0.13 = 13\%$

B atoms volume density $= \frac{1\text{ atom}}{64\text{Å}^3} = 1.56\cdot 10^{22}\frac{1}{\text{cm}^3}$

number of A atoms on (100) plane $= 4\cdot\frac{1}{4} = 1$

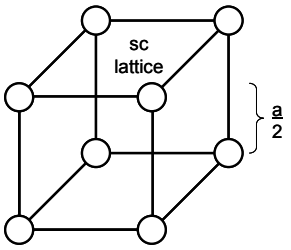
A atoms (100) aerial density $= \frac{1\text{ atom}}{(4\text{Å})^2} = 6.25\cdot 10^{14}\frac{1}{\text{cm}^2}$

Prob. 1.13

Find atoms/cell and nearest neighbor distance for sc, bcc, and fcc lattices.

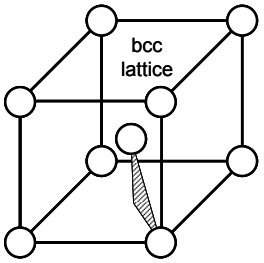
sc: atoms/cell $= 8 \cdot \frac{1}{8} = 1$

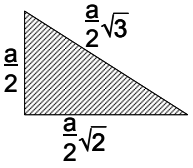
nearest neighbor distance $= a$



bcc: atoms/cell $= 8 \cdot \frac{1}{8} + 1 = 2$

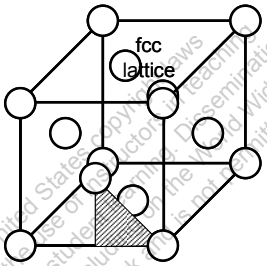
nearest neighbor distance $= \frac{a \cdot \sqrt{3}}{2}$

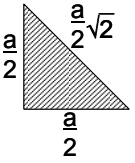




fcc: atoms/cell $= 8 \cdot \frac{1}{8} + 6 \cdot \frac{1}{2} = 4$

nearest neighbor distance $= \frac{a \cdot \sqrt{2}}{2}$

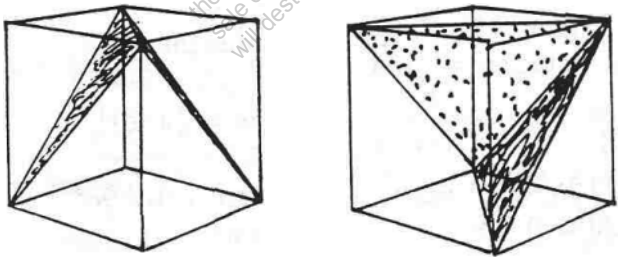




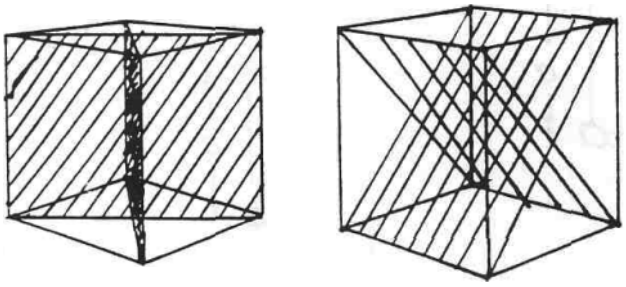
Prob. 1.14

Draw cubes showing four {111} planes and four {110} planes.

{111} planes



{110} planes



Prob. 1.15

Find fraction occupied for sc, bcc, and diamond lattices.

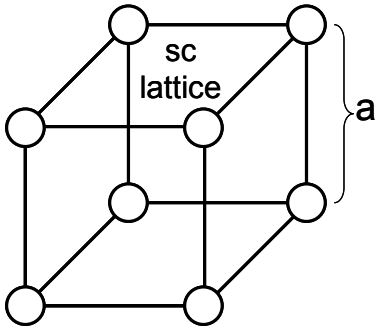
sc: atoms/cell $= 8 \cdot \frac{1}{8} = 1$

nearest neighbor = a → radius $= \frac{a}{2}$

atom sphere volume $= \frac{4\pi}{3} \cdot \left(\frac{a}{2}\right)^3 = \frac{\pi \cdot a^3}{6}$

unit cell volume $= a^3$

fraction occupied $= \frac{1 \cdot \frac{\pi \cdot a^3}{6}}{a^3} = \frac{\pi}{6} = 0.52$



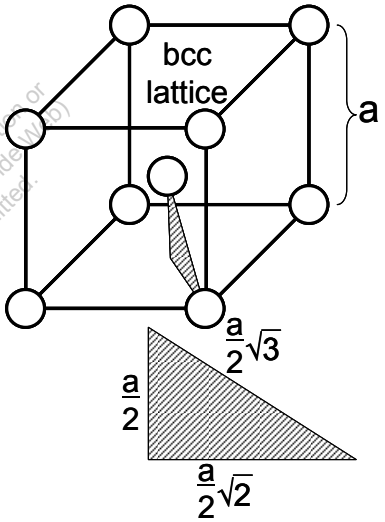
bcc: atoms/cell $= 8 \cdot \frac{1}{8} + 1 = 2$

nearest neighbor $= \frac{a \cdot \sqrt{3}}{2}$ → radius $= \frac{a \cdot \sqrt{3}}{4}$

atom sphere volume $= \frac{4\pi}{3} \cdot \left(\frac{a \cdot \sqrt{3}}{4}\right)^3 = \frac{\pi \cdot \sqrt{3} \cdot a^3}{16}$

unit cell volume $= a^3$

fraction occupied $= \frac{2 \cdot \frac{\pi \cdot \sqrt{3} \cdot a^3}{16}}{a^3} = \frac{\pi \cdot \sqrt{3}}{8} = 0.68$



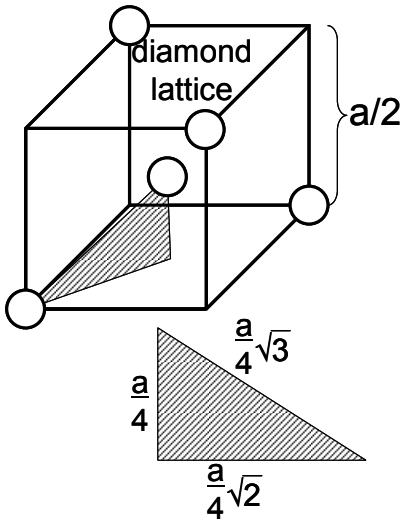
diamond: atoms/cell = 4 (fcc) + 4 (offset fcc) = 8

nearest neighbour $= \frac{a \cdot \sqrt{3}}{4}$ → atom radius $= \frac{a \cdot \sqrt{3}}{8}$

atom sphere volume $= \frac{4\pi}{3} \cdot \left(\frac{a \cdot \sqrt{3}}{8}\right)^3 = \frac{\pi \cdot \sqrt{3} \cdot a^3}{128}$

unit cell volume $= a^3$

fraction occupied $= \frac{8 \cdot \frac{\pi \cdot \sqrt{3} \cdot a^3}{128}}{a^3} = \frac{\pi \cdot \sqrt{3}}{16} = 0.34$



Prob. 1.16

Calculate densities of Ge and InP.

The atomic weights of Ge, In, and P are 72.6, 114.8, and 31, respectively.

Ge: $a = 5.66 \cdot 10^{-8}$ cm, 8 atoms/cell

$$\frac{8 \text{ atoms}}{a^3} = \frac{8}{\left(5.66 \cdot 10^{-8} \text{cm}\right)^3} = 4.41 \cdot 10^{22} \frac{1}{\text{cm}^3}$$

$$\text{density} = \frac{4.41 \cdot 10^{22} \frac{1}{\text{cm}^3} \cdot 72.6 \frac{\text{g}}{\text{mol}}}{6.02 \cdot 10^{23} \frac{1}{\text{mol}}} = 5.32 \frac{\text{g}}{\text{cm}^3}$$

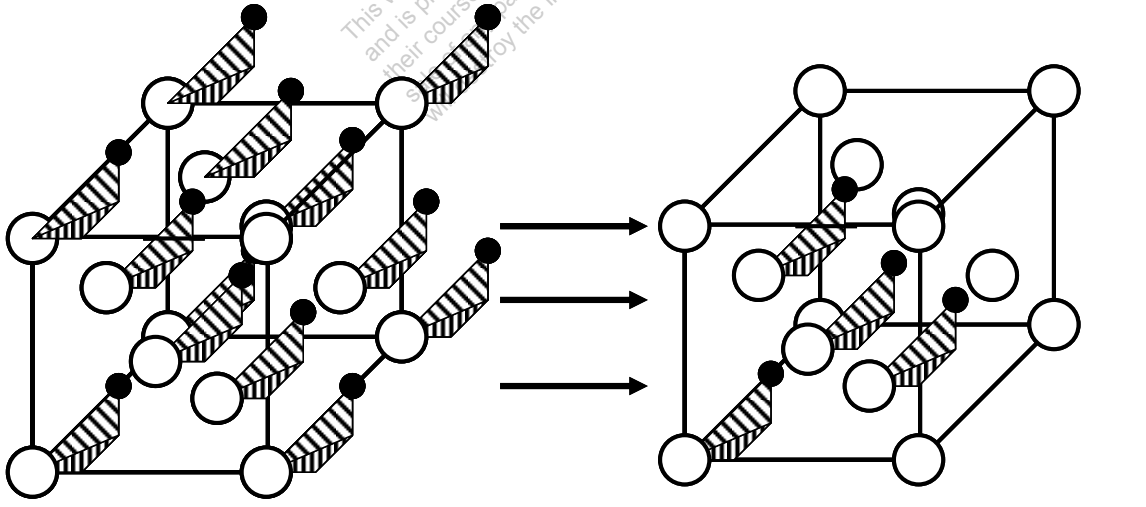
GaAs: $a = 5.87 \cdot 10^{-8}$ cm, 4 each In, P atoms/cell

$$\frac{4}{a^3} = \frac{4}{\left(5.87 \cdot 10^{-8} \text{cm}\right)^3} = 1.98 \cdot 10^{22} \frac{1}{\text{cm}^3}$$

$$\text{density} = \frac{1.98 \cdot 10^{22} \frac{1}{\text{cm}^3} \cdot \left(114.8 + 31\right) \frac{\text{g}}{\text{mol}}}{6.02 \cdot 10^{23} \frac{1}{\text{mol}}} = 4.79 \frac{\text{g}}{\text{cm}^3}$$

Prob. 1.17

Sketch diamond lattice showing four atoms of interpenetrating fcc in unit cell..



Full Interpenetrating Lattice Four Interpenetrating Atoms in Unit Cell

Prob. 1.18

Find $AlSb_xAs_{1-x}$ to lattice match InP and give band gap.

Lattice constants of AlSb, AlAs, and InP are 6.14Å, 5.66Å, and 5.87Å, respectively from Appendix III. Using Vegard's Law,

$$6.14\text{Å} \cdot x + 5.66\text{Å} \cdot (1 - x) = 5.87\text{Å} \rightarrow x = 0.44$$

$AlSb_{0.44}As_{0.56}$ lattice matches InP and has E_g=1.9eV from Figure 1-13.

Find $In_xGa_{1-x}P$ to lattice match GaAs and give band gap.

Lattice constant of InP, GaP, and GaAs are 5.87Å, 5.45Å, and 5.65Å, respectively from Appendix III. Using Vegard's Law,

$$5.87\text{Å} \cdot x + 5.45\text{Å} \cdot (1 - x) = 5.65\text{Å} \rightarrow x = 0.48$$

$In_{0.48}Ga_{0.52}P$ lattice matches GaAs and has E_g=2.0eV from Figure 1-13.

Prob. 1.19

A Si crystal is to be grown by the Czochralski method, and it is desired that the ingot contain 10^{16} phosphorus atoms/cm^3.

(a) What concentration of phosphorus atoms should the melt contain to give this impurity concentration in the crystal during the initial growth? For P in Si, k_d = 0.35.

(b) If the initial load of Si in the crucible is 5 kg, how many grams of phosphorus should be added? The atomic weight of phosphorus is 31.

SOLUTION

(a) Assume that $C_S = k_d C_L$ throughout the growth. Thus the initial concentration of P in the melt should be

$$\frac{10^{16}}{0.35} = 2.86 \times 10^{16} \text{ cm}^{-3}$$

(b) The P concentration is so small that the volume of melt can be calculated from the

weight of Si. From Appendix III the density of Si is 2.33 g/cm^3. In this example we will neglect the difference in density between solid and molten Si.

$$\frac{5000 \text{ g of Si}}{2.33 \text{ g/cm}^3} = 2146 \text{ cm}^3 \text{ of Si}$$

$$2.86 \times 10^{16} \text{ cm}^{-3} \times 2146 \text{ cm}^3 = 6.14 \times 10^{19} \text{ P atoms}$$

$$\frac{6.14 \times 10^{19} \text{ atoms} \times 31 \text{ g/mole}}{6.02 \times 10^{23} \text{ atoms/mole}} = 3.16 \times 10^{-3} \text{ g of P}$$

Since the P concentration in the growing crystal is only about one-third of that in the melt, Si is used up more rapidly than P in the growth. Thus the melt becomes richer in P as the growth proceeds, and the crystal is doped more heavily in the latter stages of growth. This assumes that k_d is not varied; a more uniformly doped ingot can be grown by varying the pull rate (and therefore k_d) appropriately. Modern Czochralski growth systems use computer controls to vary the temperature, pull rate, and other parameters to achieve fairly uniformly doped ingots.