Chapter 1 Solutions (Global Edition)

<u>Prob. 1.1</u>

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

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

smallest E_g : InSb, 0.18 eV

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

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

<u>Prob. 1.2</u>

For a bcc lattice structure with a lattice constant of 3 Å, calculate the separating distance between the nearest atoms, radius, and volume of each atoms. Also find the maximum packing fraction.

$$\text{Nearest atoms at separation } = \frac{1}{2}\sqrt{3^2 + 3^2 + 3^2} = 2.598\,\text{Å}$$

$$\text{Radius of each atom } = \frac{1}{2} \times 2.598 = 1.299\,\text{Å}$$

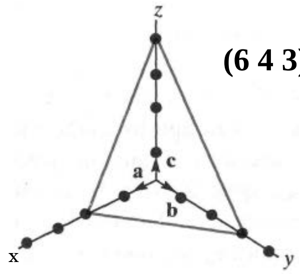
$$\text{Volume of each atom } = \frac{4}{3}\pi x (1.299)^3 = 9.18\,\text{Å}^3$$

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

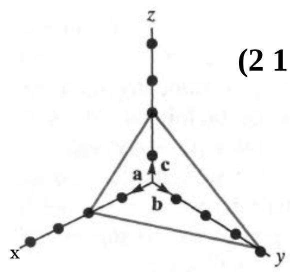
$$\text{Maximum packing fraction } = \frac{9.18 \times 2}{(3)^3} = 68\%$$

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

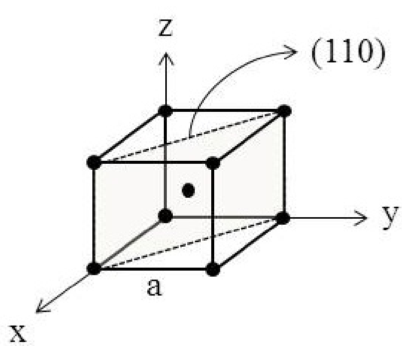
Prob.1.4

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?

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

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

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



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

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

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

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

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

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

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

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

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

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

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

Prob. 1.6

The atomic radius of Ga and As are 136 pm and 114 pm, respectively. Using hard sphere approximation, find the lattice constant of GaAs and the volume of the primitive cell. [1 Å = 100 pm]

Atomic radius of Ga = 1.36 Å and of As = 1.14 Å. Thus lattice constant will be

$$\frac{\sqrt{3}a}{4} = 1.36 + 1.14 = 2.5$$

$$a = 5.773$$

Since it has s FCC unit cell, thus volume of the primitive cell will be

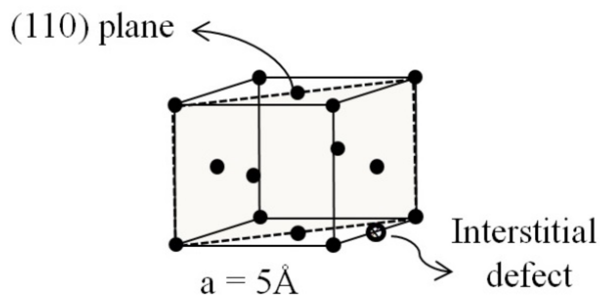
$$= \frac{a^3}{4} = 48.03 \, \text{Å}^3$$

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?

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

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



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

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

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

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

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

Volume of unit cells = a^3 = $(125)\text{Å}^3$ = 1.25×10^{-22} cm^3

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

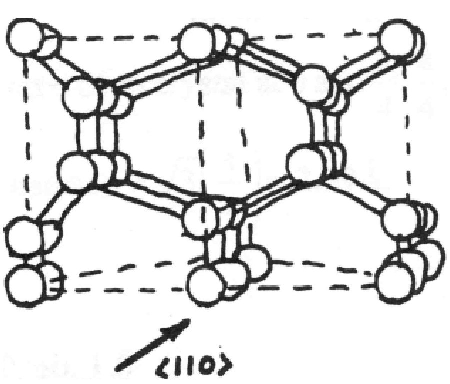
Volume density = $\frac{4}{1.25\times10^{-22}}$ atoms/cm^3

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

An interstitial defect is marked on the FCC sketch above.

Prob. 1.8

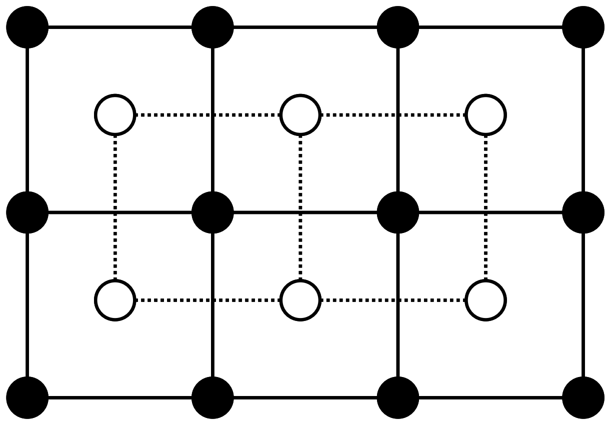
Draw <110> direction of diamond lattice.

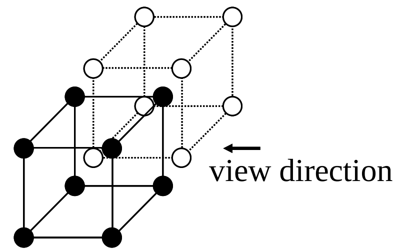


This view is tilted slightly from (110) to show the alignment of atoms. The open channels are hexagonal along this direction.

Prob. 1.9

Show bcc lattice as interpenetrating sc lattices.

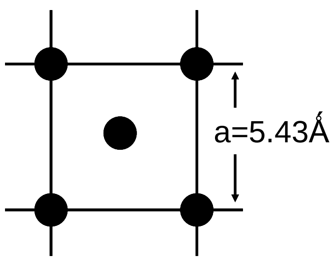




The shaded points are one sc lattice. The open points are the interpenetrating sc lattice located a/2 behind the plane of the front shaded points.

Prob. 1.10

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

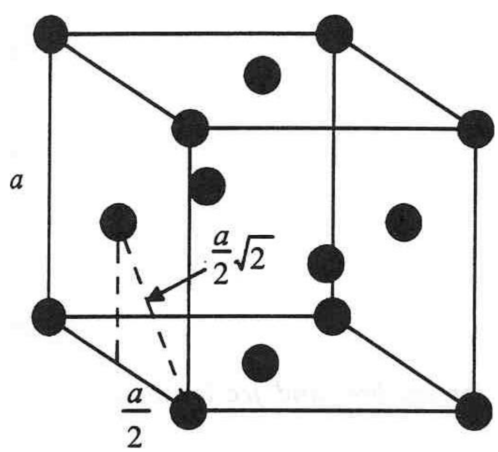


fcc lattice with a = 5.43Å

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

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

(b) Find the nearest neighbor distance in InP.



fcc lattice with a = 5.87Å

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

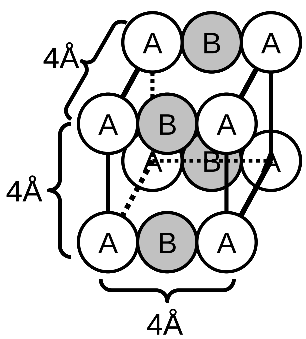
½ Na and ½ Cl atoms per unit cell $= \dfrac{\frac{1}{2}\frac{\text{atoms}}{\text{cell}}\cdot 23\frac{\text{g}}{\text{mol}} + \frac{1}{2}\frac{\text{atoms}}{\text{cell}}\cdot 35.5\frac{\text{g}}{\text{mol}}}{6.02\cdot 10^{23}\frac{\text{atoms}}{\text{mol}}} = 4.86\cdot 10^{-23}\frac{\text{g}}{\text{cell}}$

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

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 $= (4\text{Å})^3 = 64\text{Å}^3$

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

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

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

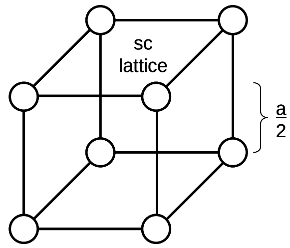
$$\text{A atoms (100) aerial density} = \frac{1\text{ atom}}{(4\text{Å})^2} = 6.25\cdot 10^{14}\frac{1}{\text{cm}^2}$$

Prob. 1.13

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

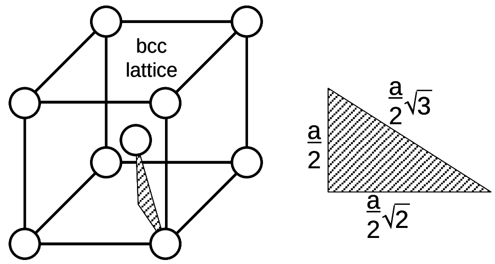
sc: atoms/cell $= 8 \cdot \frac{1}{8} = 1$

nearest neighbor distance $= a$



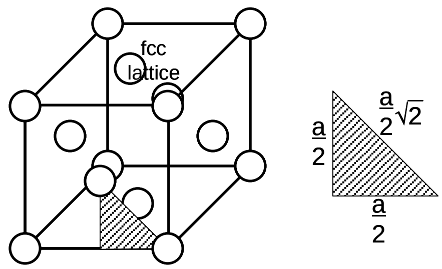
bcc: atoms/cell $= 8 \cdot \frac{1}{8} + 1 = 2$

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



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

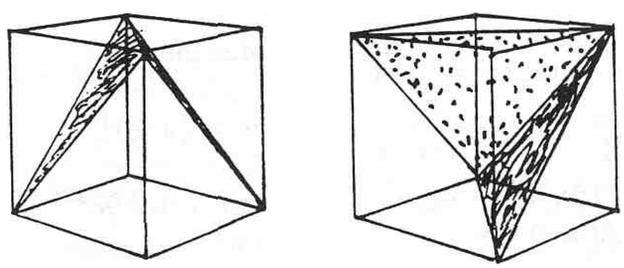
nearest neighbor distance $= \dfrac{a \cdot \sqrt{2}}{2}$



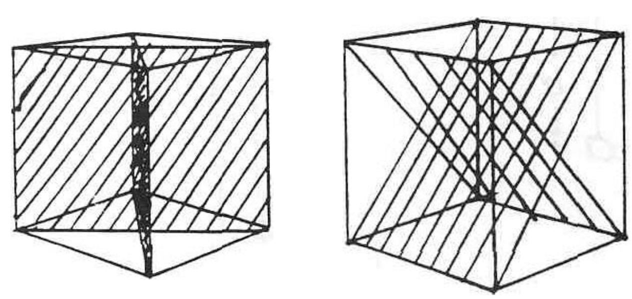
Prob. 1.14

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

{111} planes



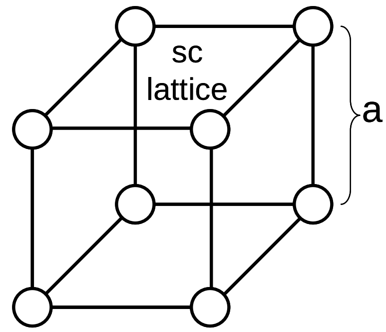
{110} planes



Prob. 1.15

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

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



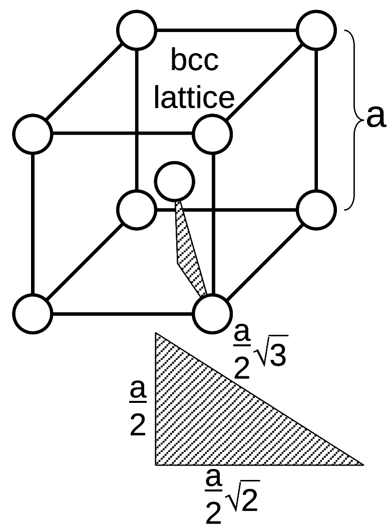
nearest neighbor $= a \rightarrow$ radius $= \dfrac{a}{2}$

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

unit cell volume $= a^3$

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

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



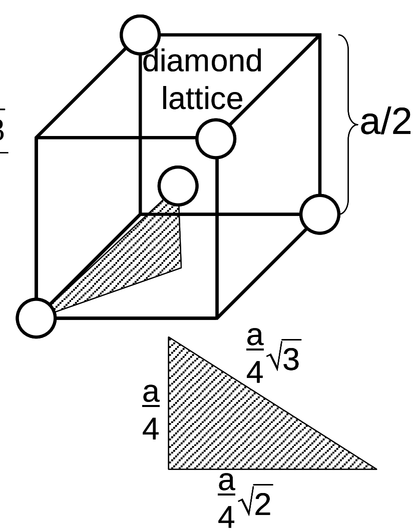
nearest neighbor $= \dfrac{a \cdot \sqrt{3}}{2} \rightarrow$ radius $= \dfrac{a \cdot \sqrt{3}}{4}$

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

unit cell volume $= a^3$

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

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



nearest neighbour $= \dfrac{a \cdot \sqrt{3}}{4} \rightarrow$ atom radius $= \dfrac{a \cdot \sqrt{3}}{8}$

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

unit cell volume $= a^3$

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

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

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

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

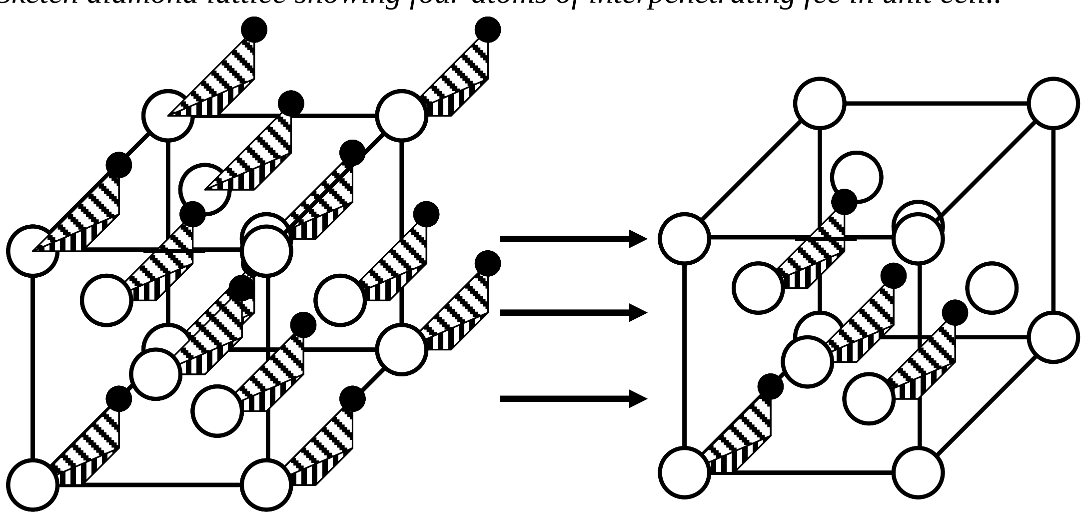
GaAs: $a = 5.87 \cdot 10^{-8}$ cm, 4 each In, P atoms/cell

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

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

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) Find the composition of In1-xGaxAs grown lattice-matched on InP substrate. The lattice constants are: a(InAs) = 6.0584 Å, a(GaAs) = 5.6533 Å, and a(InP) = 5.8688 Å.

B) An alloy of In0.2Ga0.8As is grown pseudomorphically on a GaAs substrate. Determine the maximum thickness of the grown layer.

SOLUTION

A) The lattice matching condition for $In_{1-x}Ga_xAs$ grown on an InP substrate is $(1-x)a_{\text{InAs}} + xa_{\text{GaAs}} = a_{\text{InP}}$. This gives (1-x). 6.0584 + x. 5.6533 = 5.8688. Solving x = 0.47.

The composition is $In_{0.53}Ga_{0.47}As$.

B) The lattice constant of $In_{0.2}Ga_{0.8}As$ is 0.2x6.0584 + 0.8x5.6533 = 5.7343 Å. The strain is ε = [*a* (InGaAs)-*a*(GaAs)]/*a*(GaAs) = 0.0143. The critical layer thickness is $h_c \approx a(GaAs)/2|\varepsilon|$ = 198 Å.

Therefore the maximum thickness of the pseudomorphically grown InGaAs alloy layer is 198 Å.