

## Chapter 1

### Prob. 1.1

Which semiconductor in Table I-1 has the largest  $E_g$ ? the smallest? What is the corresponding  $\lambda$ ? 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.

$$\lambda = 6.89 \mu\text{m}$$

Note Al compounds have larger  $E_g$  than the corresponding Ga compounds, which are larger than In compounds.

### Prob. 1.2

Here we need to calculate the maximum packing fraction, treating the atoms as hard spheres.

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

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

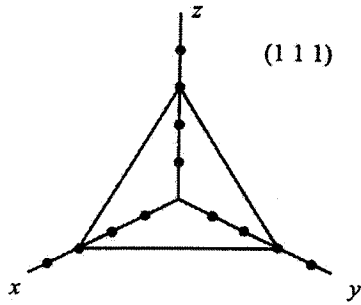
$$\text{Volume of each atom} = \frac{4}{3} \pi (2.165)^3 = 42.5 \text{ \AA}^3$$

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

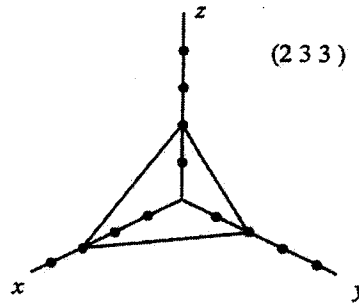
$$\text{Packing fraction} = \frac{42.5 \times 2}{(5)^3} = 68\%$$

**Prob. 1.3**

(a) Label planes:

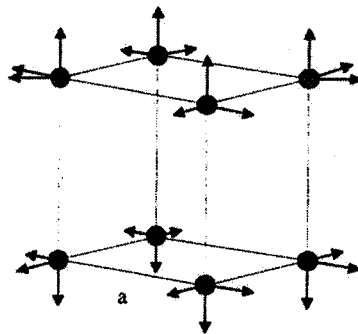


$$\begin{array}{ccc} x & y & z \\ \hline 3 & 3 & 3 \\ 1/3 & 1/3 & 1/3 \\ 1 & 1 & 1 \end{array}$$

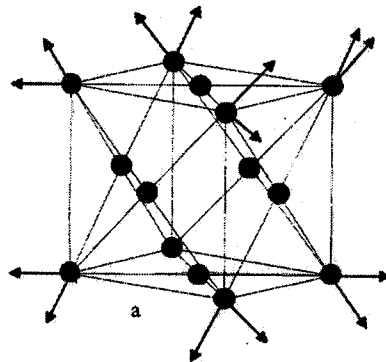


$$\begin{array}{ccc} x & y & z \\ \hline 3 & 2 & 2 \\ 1/3 & 1/2 & 1/2 \\ 2 & 3 & 3 \end{array}$$

(b) Draw equivalent directions in a cube

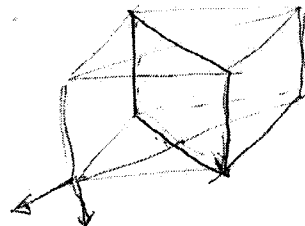


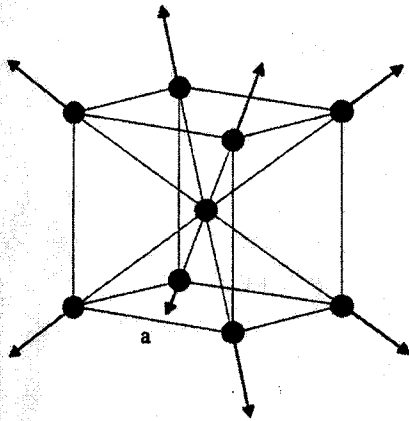
$\langle 100 \rangle$  all edges



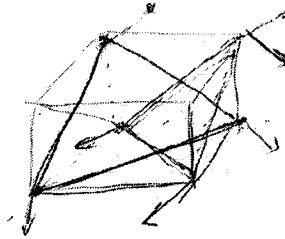
$\langle 110 \rangle$  all face diagonals

(Need not show atoms)





$\langle 111 \rangle$  all body diagonals



**Prob. 1.4**

We need to calculate the volume density of Si, its density on the (110) plane and the distance between two adjacent (111) planes.

Si FCC lattice with basis of 2 atoms

$$\text{Number of atoms per cube} = \left( 8 \times \frac{1}{8} + \frac{1}{2} \times 6 \right) \times 2 = 8$$

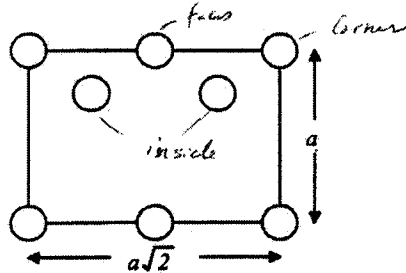
$$\text{Density} = \frac{8 \cdot m_{\text{Si}}}{(5.43 \times 10^{-8})^3} = 5.00 \times 10^{22} \text{ cm}^{-3}$$

Diamond lattice

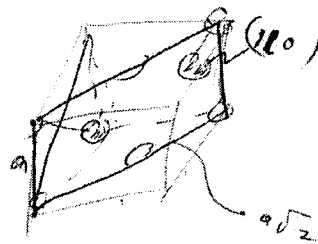
$$8\left(\frac{1}{8}\right) + 6\left(\frac{1}{2}\right) + 4 = 8$$

'corner face inside atoms

On the (110) plane we have 4 atoms on corners, 2 on the top and bottom planes, and 2 interior (see Fig. 1-a).



$$\left(\frac{1}{4}\right) 4 + \frac{1}{2}(2) + 2 = 4$$



$$(110) \text{ plane: } \frac{4 \times \frac{1}{4} + \frac{1}{2} \times 2 + 2}{(5.43 \times 10^{-8})(\sqrt{2} \times 5.43 \times 10^{-8})} = 9.59 \times 10^{14} \text{ cm}^{-2} \quad \checkmark$$

Basis of Si crystal at  $0$  and  $\frac{a}{4}, \frac{a}{4}, \frac{a}{4}$  which is along  $[111]$ .

$$\text{Distance} = \sqrt{3} \left( \frac{a}{4} \right) = 2.39 \text{ \AA}.$$

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

**Prob. 1.5**

Using the hard-sphere model, find the lattice constant of InSb, the volume of the primitive cell and the atomic density on the (110) plane.

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

$$a = 6.47 \text{ \AA}$$

In FCC, unit cell has 4 lattice points. Therefore, volume of primitive cell =  $\frac{a^3}{4} = 67.7 \text{ \AA}^3$

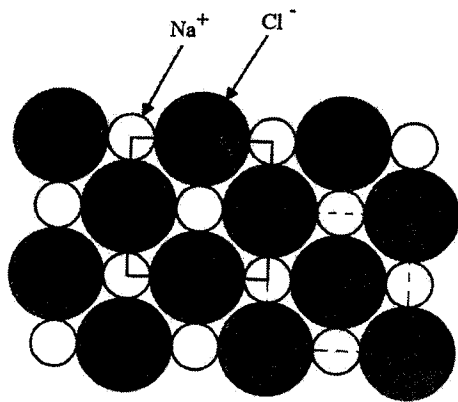
$$\text{Area of (110) plane} = \sqrt{2}a^2$$

$$\text{Density of In atoms} = \frac{4 \times \frac{1}{4} + 2 \times \frac{1}{2}}{\sqrt{2}a^2} = \frac{\sqrt{2}}{a^2} = 3.37 \times 10^{14} \text{ cm}^{-2}$$

$$\text{Same number of Sb atoms} = 3.37 \times 10^{14} \text{ cm}^{-2}$$

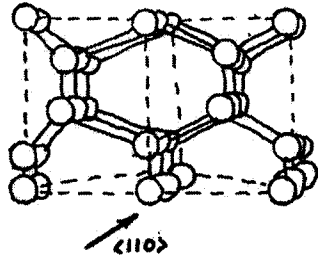
**Prob. 1.6**

*Draw NaCl lattice (1 0 0) and unit cell.*



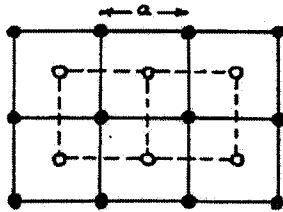
Two possible unit cells are shown, with either Na<sup>+</sup> or Cl<sup>-</sup> at the corners.

Prob. 1.7

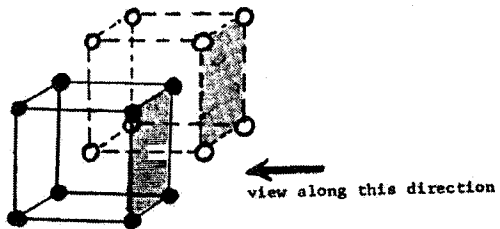


This view is tilted slightly from  $\langle 110 \rangle$  to show the alignment of atoms. The open channels are hexagonal along this direction.

Prob. 1.8

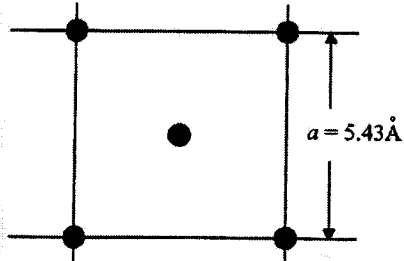


The shaded points are one sc lattice; the open points are the interpenetrating sc, located  $a/2$  behind the plane of the front shaded points.



**Prob. 1.9**

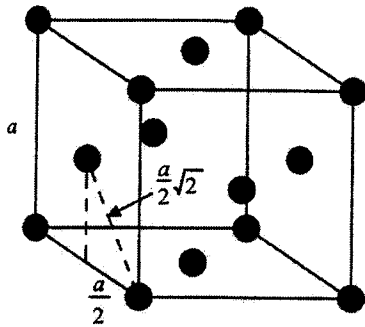
(a) Find the number of Si atoms/cm<sup>2</sup> on the surface of a (1 0 0) oriented Si wafer.



Each  $a^2$  has  $1 + \frac{1}{4}(4) = 2$  atoms on the surface.

$$\frac{2 \text{ atoms/cell}}{(5.43 \times 10^{-8})^2 \text{ cm}^2/\text{cell}} = 6.78 \times 10^{14} \text{ cm}^{-2}$$

(b) What is the distance (in Å) between nearest In neighbors in InP?



In atoms are in an fcc sublattice with  $a = 5.87 \text{ \AA}$ , nearest neighbors are

$$\frac{a}{2} \sqrt{2} = \frac{5.87}{2} \sqrt{2} = 4.15 \text{ \AA}$$

$$\sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2} = \frac{a}{2} \sqrt{2}$$

**Prob. 1.10**

Find NaCl density.

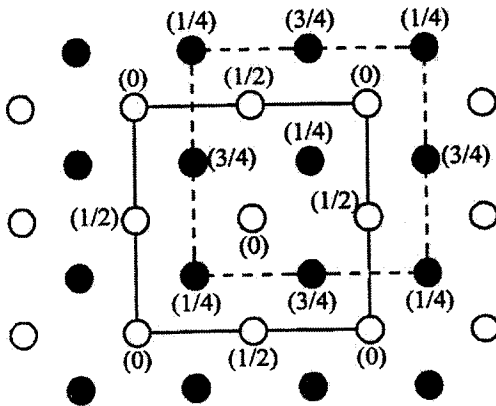
Na<sup>+</sup>: atomic wt. 23, radius 1 Å. Cl<sup>-</sup>: atomic weight 35.5, radius 1.8 Å.

The unit cell contains ½ Na and ½ Cl atoms. Using the hard sphere approximation, a = 2.8 Å.

$$\text{density} = \frac{\frac{1}{2}(23 + 35.5)/(6.02 \times 10^{23})}{(2.8 \times 10^{-8})^3} = 2.2 \text{ g/cm}^3$$

**Prob. 1.11**

Label atom planes in Fig. 1.8b.



**Prob. 1.12**

Find atoms/cell and nearest neighbor distance for sc, bcc, and fcc lattices. (see solution to Prob. 1.5)

for sc

$$\begin{aligned} \text{atoms/cell} &= \frac{1}{8}(8) = 1 \\ \text{nearest neighbor} &= a \end{aligned}$$

for bcc

$$\begin{aligned} \text{atoms/cell} &= \frac{1}{8} + 1 = 2 \\ \text{nearest neighbor} &= \frac{a}{2}\sqrt{3} \end{aligned}$$

for fcc

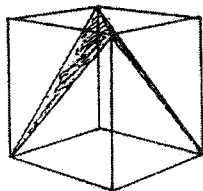
(see Example 1-1)

$$\begin{aligned} \text{atoms/cell} &= 4 \\ \text{nearest neighbor} &= \frac{1}{2}a\sqrt{2} \end{aligned}$$

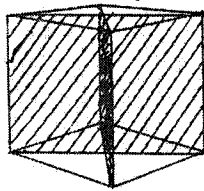


**Prob. 1.13**

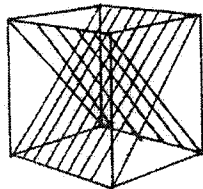
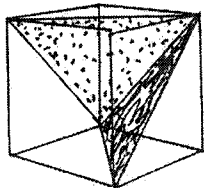
Show four  $\{111\}$  planes. Repeat for  $\{110\}$  planes.



$\{111\}$

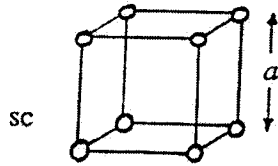


$\{110\}$

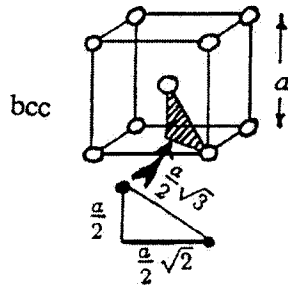


**Prob. 1.14**

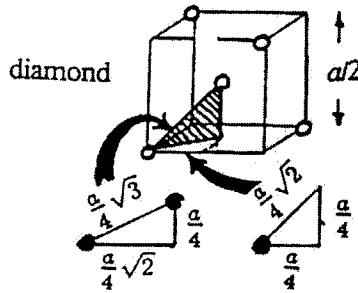
Find fraction occupied in sc, bcc, diamond.



atoms/cell =  $\frac{1}{8}(8) = 1$   
 nearest neighbor distance =  $a$   
 maximum sphere radius =  $a/2$   
 vol. of each sphere =  $\frac{4}{3}\pi(\frac{a}{2})^3$   
 total occupied vol. =  $1 \text{ atom/cell} \times \frac{\pi}{6}a^3$   
 vol. of unit cell =  $a^3$   
 fraction occupied =  $\frac{\pi}{6} = 0.52$



2 atoms/cell  
 nearest neighbor distance =  $\frac{a}{2}\sqrt{3}$   
 $r_{max} = \frac{a}{4}\sqrt{3}$   
 fraction occupied =  $(\frac{4}{3}\pi(\frac{a}{4}\sqrt{3})^3 \times 2)/a^3$   
 $= \frac{\pi}{8}\sqrt{3} = 0.68$



8 atoms/cell (4 from fcc +  
 4 at  $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$  from fcc atoms)  
 nearest neighbor distance =  $\frac{a}{4}\sqrt{3}$   
 $r_{max} = \frac{a}{8}\sqrt{3}$   
 fraction occupied =  $(\frac{4}{3}\pi(\frac{a\sqrt{3}}{8})^3 \times 8)/a^3$   
 $= \frac{\pi}{16}\sqrt{3} = 0.34$

**Prob. 1.15**

Find Ge and InP densities as in Example 1-3.

The atomic weight of Ge is 72.6; for In, 114.8; for P, 31.

For Ge:  $a = 5.66\text{\AA}$ , 8 atoms per cell

$$\frac{8}{a^3} = \frac{8}{(5.66 \times 10^{-8})^3} = 4.41 \times 10^{22} \text{ atoms/cm}^3$$

$$\text{density} = \frac{4.41 \times 10^{22} \times 72.6}{6.02 \times 10^{23}} = 5.32 \text{ g/cm}^{-3}$$

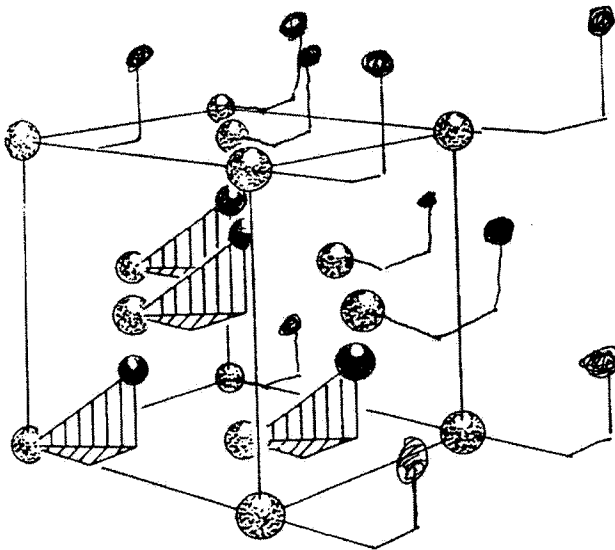
For InP:  $a = 5.87\text{\AA}$ , 4 In + 4 P per cell

$$\frac{4}{a^3} = \frac{4}{(5.87 \times 10^{-8})^3} = 1.98 \times 10^{22} \text{ atoms/cm}^3$$

$$\text{density} = \frac{1.98 \times 10^{22} \times (114.8 + 31)}{6.02 \times 10^{23}} = 4.79 \text{ g/cm}^{-3}$$

**Prob. 1.16**

Sketch diamond lattice and show only four atoms in the interpenetrating fcc are in the unit cell.



**Prob. 1.17**

What composition of  $AlSb_xAs_{1-x}$  is lattice matched to  $InP$ ?  $InGaP$  to  $GaAs$ ?  
What are the  $E_g$ 's?

From Fig. 1-15  $AlSb_xAs_{1-x}$  ternary crosses the  $InP$  lattice constant at  $x = 0.43$  where  $E_g = 1.9$  eV

$In_xGa_{1-x}P$  crosses the  $GaAs$  lattice constant at  $x = 0.48$ , where  $E_g = 2$  eV

**Prob. 1.18**

What weight of  $As$  ( $k_d = 0.3$ ) should be added to 1 kg  $Si$  to achieve  $10^{15} cm^{-3}$  doping during initial Czochralski growth?

The atomic weight of  $As$  is 74.9. *3/mole*

$$C_s = k_d C_L, \text{ thus } C_L = 10^{15} / 0.3 = 3.33 \times 10^{15} cm^{-3}$$

Calculating the melt volume from the weight of  $Si$  only, and neglecting the difference in density for solid and molten  $Si$ ,

$$\frac{1000 \text{ g of } Si}{2.33 \text{ g/cm}^3} = 429.2 \text{ cm}^3 \text{ of } Si$$

$$3.33 \times 10^{15} cm^{-3} \times 429.2 cm^3 = 1.43 \times 10^{18} \text{ As atoms}$$

$$\frac{1.43 \times 10^{18} \times 74.9 \text{ } \overset{\text{3/mole}}{\text{atoms}}}{6.02 \times 10^{23} \text{ } \overset{\text{atoms}}{\text{mole}}} = 1.8 \times 10^{-4} \text{ g} = 1.8 \times 10^{-7} \text{ kg of As.}$$