Solution for Exercise-sheet 1

I. Space lattices

(I.1) Primitive and unit cell
(1) The unit cells are A,B,C,D, and F.
(2) The primitive cells are C,D, and F.

(I.2)
(a) face-centered cubic (fcc) unit cell
A sphere at corner of fcc unit cell shares the volume with 8 unit cells. Therefore the number of spheres at the corner is 1/8. There is 8 corners in the fcc unit cell. A sphere at the face shares with 2 unit cells, i.e., the number is 1/2. There are 6 faces in the fcc unit cell. The total number of the spheres is then $\frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$.
(b) body-centered cubic (bcc)
$\frac{1}{8} \times 8 + 1 = 2$
(c) diamond
$\frac{1}{8} \times 8 + \frac{1}{2} \times 6 + 4 = 8$
Note: The diamond unit cell consists of 4 bcc unit cells. Therefore the number of atoms is 4 times the bcc value.

(I.3)
Density $= \frac{N}{V}$, where the N is the number of atoms in the unit cell and V is the volume of the unit cell.
(a)$\frac{1}{a^3} = \frac{1}{(5\times10^{-8})^3} = 8 \times 10^{21}$[atoms/cm^3]
(b)$\frac{2}{a^3} = \frac{1}{(5\times10^{-8})^3} = 1.6 \times 10^{22}$[atoms/cm^3]
(c)$\frac{4}{a^3} = \frac{4}{(5\times10^{-8})^3} = 3.2 \times 10^{22}$[atoms/cm^3]

(I.4)
(a) The diamond structure
(b) (8 atoms) / (the volume of $(5.45 \times 10^{-8})^3$)=4.94×10^{22}atoms/cm^3

(I.5) (a) GaAs has the zincblende structure and has 4 Ga atoms per unit cell.
Density $= \frac{4}{(5.65\times10^{-8})^3} = 2.22 \times 10^{22}$[atoms/cm^3]
The same for the As atoms.
(b) Ge has the diamond structure and has 8 Ge atoms per unit cell.
Density $= \frac{8}{(5.65\times10^{-8})^3} = 4.44 \times 10^{22}$[atoms/cm^3]

(I.6)
(a) simple cubic
Assume that the lattice constant is a. Radius r of the sphere atom touching the nearest neighbor is $\frac{a}{2}$. Hence the volume of one atom V_{atom} is $\frac{4\pi}{3}(\frac{a}{2})^3$. Number of the atom n in the unit cell of cubic crystal is then 1 ($\frac{1}{8} \times 8$). The percentage of the total unit cell (density of atoms) $\%_{volume}$ can be obtained by

$$\%_{volume} = V_{atom} \times n/a^3 = \frac{\pi}{6} = 52.4\% \tag{1}$$

(b) fcc

Similarly, $r = \frac{\sqrt{2}}{4}a$, $n = 4$ (question 1.1 (a)). Therefore,

$$\%_{volume} = V_{atom} \times n/a^3 = \frac{4\pi}{3}(\frac{\sqrt{2}}{4}a)^3 \times 4/a^3 = 0.740 = 74\% \tag{2}$$

(c) bcc
$r = \frac{\sqrt{3}}{4}a$ and $n = 2$ (question 1.1 (b)). Therefore,

$$\%_{volume} = V_{atom} \times n/a^3 = \frac{4\pi}{3}(\frac{\sqrt{3}}{4}a)^3 \times 2/a^3 = 0.68 = 68\% \tag{3}$$

(d) diamond
The smallest distance between the atoms is the distance between the corner and the middle in the "tetrahedron" (figure 1.11, page 10 of Neaman book). The half of the distance, that is the radius r, is $\frac{\sqrt{3}}{8}a$. Furthermore $n = 8$ (question 1.1 (b)).

$$\%_{volume} = V_{atom} \times n/a^3 = \frac{4\pi}{3}(\frac{\sqrt{3}}{8}a)^3 \times 8/a^3 = \frac{\pi\sqrt{3}}{16} = 34\% \tag{4}$$

(I.7)
(a) The smallest distance between atoms is $\frac{\sqrt{3}}{4}a$ (the answer for the question above). Using the lattice constant gives a=2.35Å
(b) (8 atoms) / (the volume of $(5.43 \times 10^{-8})^3$)=5.0×10^{22}atoms/cm^3
(c) Mass per atom is 28.06 amu = 4.66×10^{-26} kg. Multiply the value with the density of atoms (the answer above) results 2.33g/cm^3

(I.8) See the figures 1 and 2.

(I.9)
(a) [100] plane of the Si has 2 atoms $(1/4 \times 4 + 1)$ in the unit cell with the area of a^2, where a is the lattice constant. Surface density D is then $2/(5.43 \times 10^{-8})^2 = 6.78 \times 10^{14}$atoms/cm^2
(b)[110] plane of the Si has 4 atoms $(2+1/2\times2+1/4\times4)$ in the unit cell with the area of $a \times \sqrt{2}a$. Surface density D is then $4/(\sqrt{2}5.43 \times 10^{-8})^2 = 9.59 \times 10^{14}$atoms/cm^2
(c)[111] plane of the Si has 2 atoms $(3 \times 1/2 + 3 \times 1/6)$ in the unit cell with the area of an equilateral (a regular) triangle with the side length of $\sqrt{2}a$. Surface density D is then $2/(1/2\times\sqrt{3}a^2) = 7.83 \times 10^{14}$atoms/cm^2

II. Imperfections and impurities in solids

(II.1) (a) If 2×10^{16}cm^{-3} boron atoms are added to Si, the same amount of Si atoms will be displaced among the total Si atoms (5×10^{22}cm^{-3} from question I.3(b)).

$$\frac{2 \times 10^{16}}{5 \times 10^{22}} \times 100\% = 4 \times 10^{-5}\% \tag{5}$$

(b)Similarly for the boron atoms,

$$\frac{10^{15}}{5 \times 10^{22}} \times 100\% = 2 \times 10^{-6}\% \tag{6}$$

(II.2)
c and 0.8

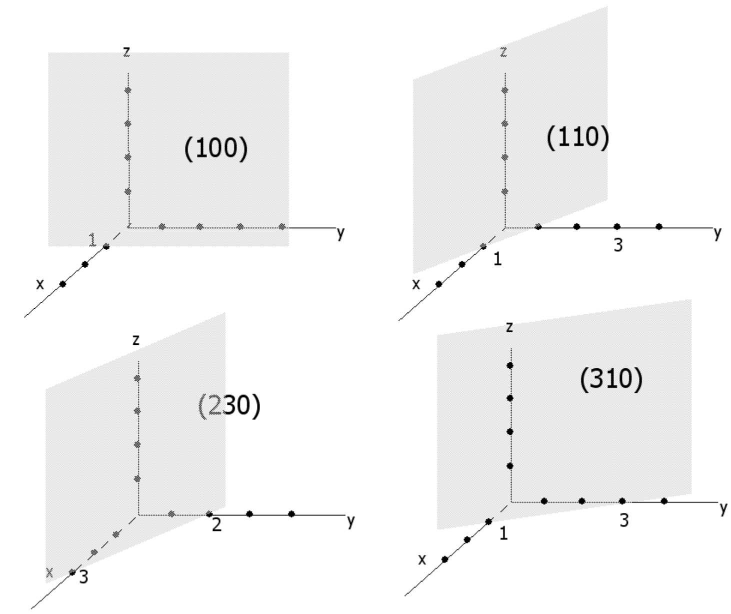

Figure 1: Crystal planes

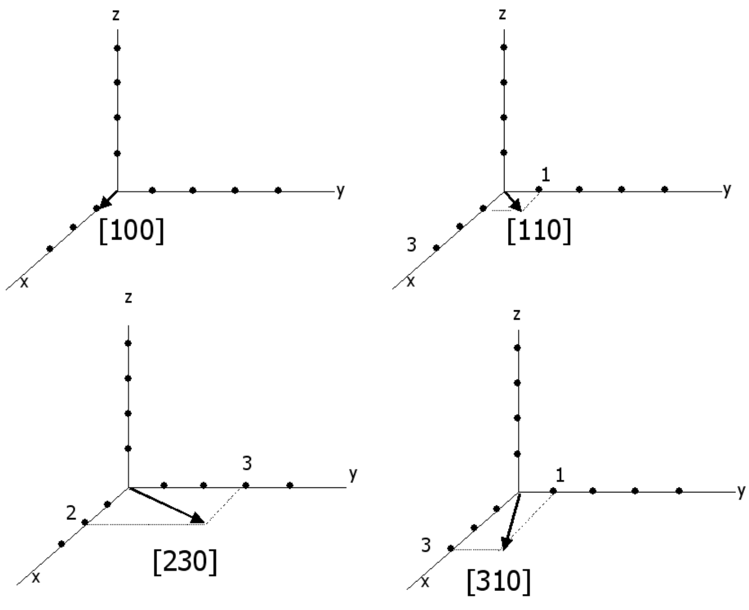

Figure 2: Crystal directions