Chapter 1 Physics and Properties of Semiconductors—A Review

1. (a) A unit cell contains 1/8 of a sphere at each corner of the eight corners, 1/2 of a sphere at each of the 6 faces, and 4 spheres inside the cell → a total of $\frac{1}{8}\times 8+\frac{1}{2}\times 6+4 = 8$ spheres. The diagonal distance between $(0, 0, 0)$ and $\left(\frac{1}{4}a, \frac{1}{4}a, \frac{1}{4}a\right)$ is $d = \sqrt{\left(\frac{a}{4}\right)^2+\left(\frac{a}{4}\right)^2+\left(\frac{a}{4}\right)^2} = \frac{a}{4}\sqrt{3}$.

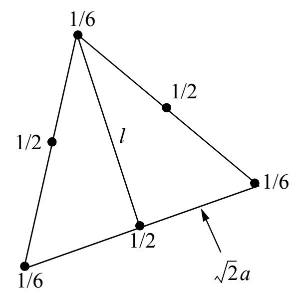
The radius of the hard sphere is $\frac{d}{2} = \frac{a}{8}\sqrt{3}$.

$$\therefore \text{ Max fraction} = \frac{8\left[\frac{4\pi}{3}\left(\frac{a}{8}\sqrt{3}\right)^3\right]}{a^3} = \frac{\pi\sqrt{3}}{16} = 34\%.$$

(b) On (111) plane

$$l = \sqrt{(\sqrt{2}a)^2-\left(\frac{\sqrt{2}a}{2}\right)^2} = \sqrt{\frac{3}{2}}a$$

$$\frac{\text{No. of atoms in }\Delta}{\text{area of }\Delta} = \frac{3\times\frac{1}{2}+3\times\frac{1}{6}}{\frac{1}{2}(\sqrt{2}a)\sqrt{\frac{3}{2}}a} = \frac{2}{\frac{\sqrt{3}}{2}a^2} = 7.83\times10^{14}\text{ atoms/cm}^2.$$

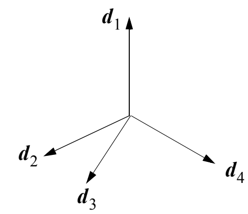


2. $\boldsymbol{d}_1+\boldsymbol{d}_2+\boldsymbol{d}_3+\boldsymbol{d}_4 = 0 \qquad |\boldsymbol{d}_1| = |\boldsymbol{d}_2| = |\boldsymbol{d}_3| = |\boldsymbol{d}_4| = d$

$$\boldsymbol{d}_1\cdot(\boldsymbol{d}_1+\boldsymbol{d}_2+\boldsymbol{d}_3+\boldsymbol{d}_4) = \boldsymbol{d}_1\cdot 0 = 0$$

$$d^2+d^2(\cos\theta_{12}+\cos\theta_{13}+\cos\theta_{14}) = d^2+3d^2\cos\theta = 0$$

$$\therefore \quad \cos\theta = -\frac{1}{3}\Rightarrow\theta = \cos^{-1}\left(-\frac{1}{3}\right) = 109.47^\circ$$



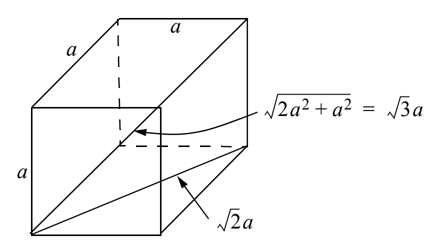
3. $V = |\boldsymbol{a}\cdot\boldsymbol{b}\times\boldsymbol{c}| = \left|\left(\frac{a}{2}, 0, \frac{a}{2}\right)\cdot\left(\frac{a}{2}, \frac{a}{2}, 0\right)\times\left(0, \frac{a}{2}, \frac{a}{2}\right)\right|$

$$= \left|\left(\frac{a}{2}, 0, \frac{a}{2}\right)\cdot\left(\begin{vmatrix}\frac{a}{2} & 0\\ \frac{a}{2} & \frac{a}{2}\end{vmatrix}, \begin{vmatrix}0 & \frac{a}{2}\\ \frac{a}{2} & 0\end{vmatrix}, \begin{vmatrix}\frac{a}{2} & \frac{a}{2}\\ 0 & \frac{a}{2}\end{vmatrix}\right)\right| = \left|\left(\frac{a}{2}, 0, \frac{a}{2}\right)\cdot\left(\frac{a^2}{4}, -\frac{a^2}{4}, \frac{a^2}{4}\right)\right| = \frac{a^3}{4}$$

4. (a)

$$d = \frac{1}{2}\sqrt{\left(\frac{a}{2}\right)^2+\left(\frac{\sqrt{2}a}{2}\right)^2}$$

$$= \frac{\sqrt{3}}{4}a$$



(b) Intercept at $2a$, $3a$ and $4a$; reciprocal: $\frac{1}{2}, \frac{1}{3}, \frac{1}{4}$. The plane is (643).

5. (a) Let R be a vector in the direct lattice, then

$$\boldsymbol{G}\cdot\boldsymbol{R} = 2\pi(hm+kn+lp) = 2\pi N$$

d = distance when the vector R coincides with G

$$= \frac{2\pi N}{|\boldsymbol{G}|}$$

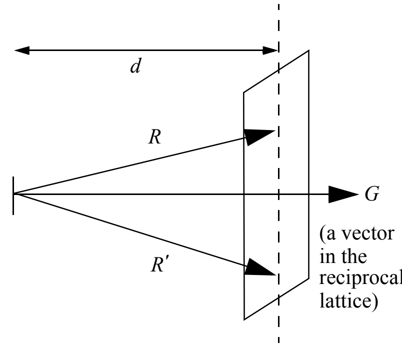
Let R' have $m' = m - Zl$, $n' = n - Zl$, and $p' = p + Z(h+k)$,

Then $\boldsymbol{G}\cdot\boldsymbol{R}' = (h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*)\cdot\{(m-Zl)\boldsymbol{a} + (n-Zl)\boldsymbol{b} + [p + Z(h+k)]\boldsymbol{c}\}$

$= (hm + kn + lp) = 2\pi N$ (same as $\boldsymbol{G}\cdot\boldsymbol{R}$)

Since $\boldsymbol{R}'$ is quite general, it can form a plane perpendicular to $\boldsymbol{G}$.

Therefore $\boldsymbol{G}$ is normal to a set of planes in the direct lattice.



(b) Volume in reciprocal lattice = $(2\pi)^3 \dfrac{(\boldsymbol{b}\times\boldsymbol{c})\cdot(\boldsymbol{c}\times\boldsymbol{a})\times(\boldsymbol{a}\times\boldsymbol{b})}{(\boldsymbol{a}\cdot\boldsymbol{b}\times\boldsymbol{c})^3} = \dfrac{(2\pi)^3}{V_C}$

6.

$$a^* = 2\pi\frac{\boldsymbol{b}\times\boldsymbol{c}}{\boldsymbol{a}\cdot\boldsymbol{b}\times\boldsymbol{c}} = 2\pi\frac{\left[\frac{a}{2}(\boldsymbol{z}+\boldsymbol{x})\right]\times\left[\frac{a}{2}(\boldsymbol{x}+\boldsymbol{y})\right]}{\left[\frac{a}{2}(\boldsymbol{y}+\boldsymbol{z})\right]\cdot\left[\frac{a}{2}(\boldsymbol{z}+\boldsymbol{x})\right]\times\left[\frac{a}{2}(\boldsymbol{x}+\boldsymbol{y})\right]} = \frac{4\pi}{a}\cdot\frac{(\boldsymbol{y}-\boldsymbol{x}+\boldsymbol{z})}{(\boldsymbol{y}+\boldsymbol{z})\cdot(\boldsymbol{y}-\boldsymbol{x}+\boldsymbol{z})} = \frac{4\pi}{a}\cdot\frac{(\boldsymbol{y}-\boldsymbol{x}+\boldsymbol{z})}{(1+1)}$$

$$= \frac{4\pi}{a}\frac{1}{2}(\boldsymbol{y}+\boldsymbol{z}-\boldsymbol{x}) \rightarrow \frac{4\pi}{a} \quad \text{(one of the vectors for bcc)}$$

Similarly, for b^* and c^*. $\therefore$ Reciprocal of fcc is bcc.

7. $\because\ E = \dfrac{k_x^2}{m_l} + \dfrac{k_y^2}{m_t} = \text{constant} = C$

Let $k_x = 0$, $\therefore\ \dfrac{k_y^2}{m_t} = C$

Let $k_y = 0$, $\therefore\ \dfrac{k_x^2}{m_l} = C$ $\quad\therefore\ \dfrac{k_y^2/m_t}{k_x^2/m_l} = 1$ $\quad\therefore\ \dfrac{m_l^*}{m_t} = \dfrac{k_x^2}{k_y^2} = \left(\dfrac{5}{1}\right)^2 = 25$

8. Ratio $= \dfrac{\left(\frac{6}{2}\right)(1.0)^{3/2}}{1(0.1)^{3/2}} = 3(10)^{3/2} = 94.8$

9. For a three dimensional structure such as a bulk semiconductor, to calculate the electron and hole concentrations in the conduction and valence bands, respectively. We need to know the density of states, that is, the number of allowed energy states per unit energy per unit volume (i.e., in the unit of number of states/eV/cm^3).

When electrons move back and forth along the x-direction in a semiconductor material, the movements can be described by standing-wave oscillations. The wavelength λ of a standing wave is related to the length of the semiconductor L by

$$L/\lambda = n_x, \tag{1}$$

where n_x is an integer. The wavelength can be expressed by de Broglie hypothesis

$$\lambda = h/k_n, \tag{2}$$

where h is the Planck's constant and k_x is the momentum in the x-direction. Substituting Eq. 2 into Eq. 1 gives

$$Lk_n = hn_x. \tag{3}$$

The incremental momentum dk_x required for a unity increase in n_x is

$$Ldk_n = h\,. \tag{4}$$

For a three-dimensional cube of side L, $Ldk_xdk_ydk_z = h^3$; furthermore, The volume $dk_xdk_ydk_z$ in the momentum space for a unit cube ($L = 1$) is equal to h^3. Each incremental change in turn corresponds to a unique set of integers (n_x, n_y, n_z), which in turn corresponds to an allowed energy state. Thus, the volume in momentum space for an energy state is h^3. The figure below shows the momentum space in spherical coordinates. The volume between two concentric spheres (from k to $k + dk$) is $4\pi k^2dk$. The number of energy states contained in the volume is then $2(4\pi k^2dk)/h^3$, where the factor 2 accounts for the electron spins. The energy E of the electron (here consider only the kinetic energy) is given by

$$k = \sqrt{2m_nE}\,, \tag{5}$$

where k is the total momentum (with components k_x, k_y, and k_z in Cartesian coordinates) and m_n is the effective mass. From Eq. 5, we can substitute E for k and obtain

$$N(E)dE = \frac{8\pi k^2dk}{h^3} = 4\pi\left(\frac{2m_n}{h^2}\right)^{\frac{3}{2}}E^{\frac{1}{2}}dE \tag{6}$$

and

$$N(E) = 4\pi\left(\frac{2m_n}{h^2}\right)^{\frac{3}{2}}E^{\frac{1}{2}}\,, \tag{7}$$

where $N(E)$ is called the density of states.

The derivation of the two-dimensional density of states is almost the same. We calculate the number of k-states enclosed within an annulus of radius k to $k + dk$ instead. The area between two concentric circles is $2\pi kdk$ and the number of energy states contained in the area is $2(2\pi kdk)/h^2$. The two-dimensional density of states is then given by

$$N(E)dE = \frac{4\pi kdk}{h^2} = 4\pi\left(\frac{m_n}{h^2}\right)dE \tag{8}$$

and

$$N(E) = 4\pi\frac{m_n}{h^2} \tag{9}$$

Finally, the derivation of the one-dimensional density of states is calculated within a line. The wavelength λ of a standing wave is related to the length L of semiconductor by

$$\frac{L}{\lambda/2} = n_x\,. \tag{10}$$

The incremental momentum dk_x required for a unity increase in n_x is

$$2Ldk_x = h\,. \tag{11}$$

dk_x in momentum space for a line with unit length is h/2 and the number of energy states contained in the line is $2dk/(h/2)$. The one-dimensional density of states is

$$N(E)dE = \frac{2dk}{h/2} = 2\sqrt{\frac{2m_n}{E}}\frac{1}{h}dE \tag{12}$$

and

$$N(E) = 2\sqrt{\frac{2m_n}{E}}\frac{1}{h}\,. \tag{13}$$

10.

$$\langle KE\rangle = \frac{\int_0^\infty (E-E_C)N(E)F(E)dE}{\int_0^\infty N(E)F(E)dE} = \left.\frac{\int_0^\infty (E-E_C)(E-E_C)^{1/2}e^{-(E-E_F)/kT}dE}{\int_0^\infty (E-E_C)^{1/2}e^{-(E-E_F)/kT}dE}\right|_{E-E_C=y,\ dy=dE}$$

$$= \left.\frac{\int_0^\infty y^{3/2}e^{-y/kT}dy}{\int_0^\infty y^{1/2}e^{-y/kT}dy}\right|_{y/kT=z} = \frac{kT\int_0^\infty z^{3/2}e^{-z}dz}{\int_0^\infty z^{1/2}e^{-z}dz} = \frac{kT\,\Gamma\left(\frac{5}{2}\right)}{\Gamma\left(\frac{3}{2}\right)} = \frac{kT\left(\frac{3}{2}\right)\left(\frac{1}{2}\right)\sqrt{\pi}}{\left(\frac{1}{2}\right)\sqrt{\pi}} = \frac{3}{2}kT$$

11.

$$N_D^+ = \frac{N_D}{1+2\exp\left(\frac{E_F-E_D}{kT}\right)} \qquad (14)$$

At 77K,

$$N_C = N_C\left(\frac{77}{300}\right)^{3/2} = 2.8\times10^{19}(0.13) = 3.64\times10^{18}\ \text{cm}^{-3} \qquad (15)$$

$$kT = 0.0259\left(\frac{77}{300}\right) = 0.006648\ \text{eV} \qquad (16)$$

$$E_C-E_F = kT\ln\left[\frac{N_C}{N_D^+(T)}\right] = 0.006648\ln\left.\frac{3.64\times10^{18}}{10^{16}}\right| \quad (\text{Let } N_D = 10^{16})$$

$$= 0.00648\ln(364) = 0.0392\ \text{eV} \qquad (17)$$

From Fig. 10 in textbook, we know that for phosphorous in Si, $E_C-E_D \approx 0.045$ eV.
Thus, from Eq. 14, we have

$$N_D^+ = \frac{10^{16}}{1+2\exp\left(\frac{-0.0392+0.045}{0.006648}\right)} = \frac{10^{16}}{1+2\exp(+0.87)}$$

$$= \frac{10^{16}}{1+4.78} = 1.73\times10^{15}\ \text{cm}^{-3} \quad (< 10^{16}\ \text{cm}^{-3})$$

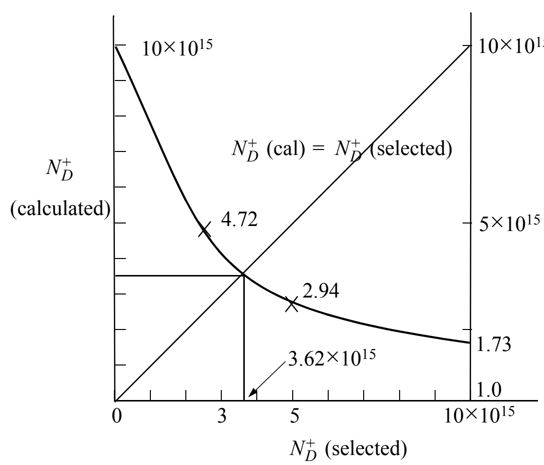
We select a new N_D^+ value, repeat the process and eventually obtain $N_D(77) \approx 3.6\times10^{15}$ cm^{-3}.

$$E_C-E_F = 0.006648\ln\left(\frac{3.64\times10^{18}}{3.6\times10^{15}}\right) \approx 0.04587\ \text{eV}$$

$$E_F-E_D = -0.00087\ \text{eV}$$

$$N_D^+ = \frac{10^{16}}{1+2e^{-0.130}} \approx \frac{10^{16}}{2.756} \approx 3.6\times10^{15}\ \text{cm}^{-3}$$

Also see the right figure.

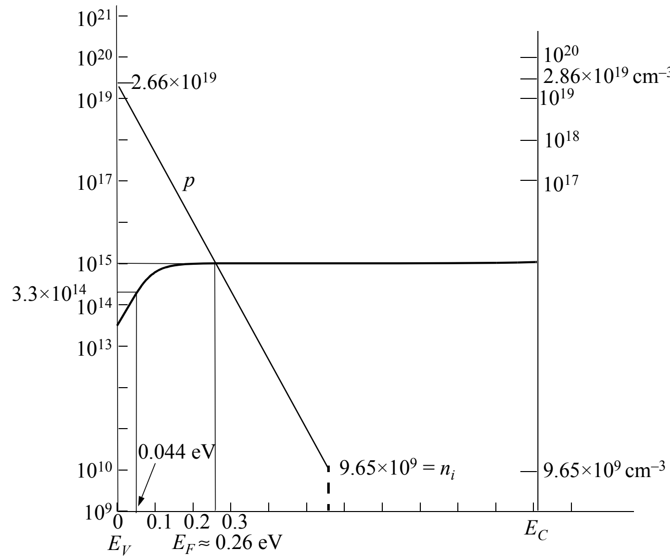


12. From Fig. 10 in textbook, $E_A - E_V = 0.044$ eV.

$$n + N_A^- = n_i e^{(E_F - E_i)/kT} + \frac{N_A}{1 + 4e^{(E_A - E_F)/kT}}$$

$$p + N_D^+ = n_i e^{(E_i - E_F)/kT} + \frac{N_D}{1 + 2e^{(E_F - E_D)/kT}} \approx p$$

Graphic result $E_F - E_V \approx 0.26$ eV, see the right diagram.



13.
$$n_{no} = \frac{1}{2}[N_D - N_A + \sqrt{(N_D - N_A)^2 + 4n_i^2}] = \frac{1}{2}[2 \times 10^{10} + \sqrt{(2\times10^{10})^2 + 4(9.3 \times 10^{19})}]$$
$$= 2.3885 \times 10^{10} \text{ cm}^{-3}$$
$$\therefore E_C - E_F = \frac{kT}{q}\ln\left(\frac{N_C}{n}\right) = 0.0259\ln\frac{2.8 \times 10^{19}}{2.39 \times 10^{10}} = 0.540 \text{ eV}$$

14. (a) $N_A \gg N_{\text{Au}}$, E_F near E_V, therefore E_A level is neutral and E_D level is positive. Therefore the state of charge of gold level is positive.

(b) No effect.

15.
$$N \propto \exp(-E_d/2kT)$$
$$\frac{10^{15}}{10^{14}} = \exp\left(\frac{-E_D}{2kT_1} + \frac{E_D}{2kT_2}\right) = \exp\left(\frac{-E_D}{0.1027} + \frac{E_D}{0.00479}\right)$$
$$54.8E_D = 2.3, \quad E_D = \frac{2.3}{54.8} = 0.041 \text{ eV}$$
. From Fig. 10 in the textbook, we know that the atom is Sb.

16.
$$E_C - E_F = kT\ln\left(\frac{N_C}{N_D}\right) = 0.0259\ln(10^3) = 0.1787 \text{ eV}$$

From Fig. 10 in the textbook, $E_C - E_D = 0.045$ eV.

$E_F - E_D = 0.045 - 0.1787$ eV $= -0.1337$; thus,

$$\frac{N_D^0}{N_D^+} = g\exp\left(\frac{E_F - E_D}{kT}\right) = 2\exp\left(-\frac{0.1337}{0.0259}\right) = 2\exp(-5.16) = \frac{2}{175.1} = 0.0114 = 1.14\%.$$