<u>Homework 7 Solutions</u>

1. Non-parabolic conduction band.

For "non-parabolic" conduction band of many semiconductors, $\frac{\hbar^2 k^2}{2m^*} = U\left(1+\alpha U\right)$

The key point is that this relationship, like the Fermi-electron U-vs-k relationship, is *spherically symmetric* in k space. So

$$N(k) = \underbrace{2}_{\text{spin}} \underbrace{\left(\frac{L}{2\pi}\right)^3}_{\text{\#states/volume in k space}} \underbrace{\tfrac{4}{3}\pi k^3}_{\text{volume of sphere}}$$ (number of states between k = 0 and k)

Solving for k^3, we get $k^3 = \left[\frac{2m^*}{\hbar^2}\right]^{3/2} \left[U\left(1+\alpha U\right)\right]^{3/2}$.

So $N(U) = \frac{V}{3\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\left[U+\alpha U^2\right]^{3/2}$

And $D(U) = \frac{dN}{dU} = \frac{V}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\left[U+\alpha U^2\right]^{1/2}\left(1+2\alpha U\right)$

Note: In the limit where $\alpha \to 0$, this gives the correct expression for a parabolic band: $D(U) \to \frac{V}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2} U^{1/2}$

2. Square lattice, free-electron energies:

(a). The wavevector at the corner is longer than the wavevector at the midpoint of a side by the factor $\sqrt{2}$. Since $U \propto k^2$ for a free electron, the energy is higher by $\left(\sqrt{2}\right)^2 = 2$.

(b). In 3D the energy is higher at a corner by $\left(\sqrt{3}\right)^2$ than at midpoint of a face.

(c). If the band gap at the midpoint of a face is less than the kinetic energy difference between this point and a corner, the electrons will spill-over into the n = 2 band in preference to filling the corner states in the n = 1 band. Divalent elements under these conditions will be metals and not insulators.

3. Kinematics of free electrons for the fcc lattice.

(a). We start with the "aliased" energy expression for the free electron, $U = \frac{\hbar^2 |\vec{k}+\vec{G}|^2}{2m}$,.

For k along the [111] direction, we can write from Kittel Chap. 2, $|\vec{k}| = \left(\frac{2\pi}{a}\right)(1,1,1)u$, with $0 < u < \frac{1}{2}$, to stay within the 1st BZ below the Nyquist wave vector. The reciprocal lattice vectors can be written as

$\vec{G} = \left(\frac{2\pi}{a}\right)\left[(h-k+l)\hat{x} + (h+k-l)\hat{y} + (-h+k+l)\hat{z}\right]$, where h, k, l are any integers.

Thus $U = \left(\frac{\hbar^2}{2m}\right)\left(\frac{2\pi}{a}\right)^2\left[(u+h-k+l)^2 + (u+h+k-l)^2 + (u-h+k+l)^2\right]$.

We now have to consider all combinations of indices h, k, l for which the term in brackets is smaller than $6\left[3(1/2)^2\right]$ = 9/2. This is done easily in Excel by trying all different permutations up to, say, h = k = l = 3, and then sorting. There are 15 resulting G vectors, specified by the Miller convention as G = (000); $(-1,-1,-1)$; $(-1,0,0)$, $(0,-1,0)$, and $(0,0,-1)$; (1,0,0), (0,1,0), and (0,0,1); (1,1,1); $(-1,-1,0)$, $(-1,0,-1)$, and $(0,-1,-1)$, (110), (101), and (011).

4. Square lattice with potential energy

As in most cases of Fourier analysis, it is best to express a real sinusoid in complex exponential form for analytic simplicity. The given form of the potential energy can be written V(x,y) = -4Vcos(2πx/a)cos(2πy/a) can be so-written (great exercise in successive use of Euler's identity: e^{jkx} = coskx + jsinkx):

$$V(x,y) = -V\left(e^{j(2\pi/a)(x+y)} + e^{j(2\pi/a)(-x+y)} + e^{j(2\pi/a)(x-y)} + e^{j(2\pi/a)(-x-y)}\right)$$

This makes it clear that Fourier decomposition of $V(\vec{r}) = \sum_G V_G\, e^{j\vec{G}\cdot\vec{r}}$ will have four Fourier components (assuming as always that $V_{G=0} = 0$), *but they all equal* -V. In setting up the central equation, we note that at the corner (Nyquist) point of the square lattice the Fourier component of the Bloch wave function is $C_k = C_{\pi/d,\pi/d}$ But there will be strong Bragg scattering at this point and hence strong excitation of the reverse traveling wave, $C_{k-G} = C_{-\pi/d,-\pi/d}$. Hence, although there are four significant G vectors $\left(\frac{2\pi}{a}\right)(\pm1;\pm1)$ there are only two significant C_k components in the central equation. Thus, in the notation of Prof. Brown's notes

$$\begin{pmatrix} W_{\vec{k}-\vec{G}_1} & V_{\vec{G}_1} \\ V_{\vec{G}_1} & W_{\vec{k}} \end{pmatrix}\begin{bmatrix} C_{\vec{k}-\vec{G}_1} \\ C_{\vec{k}} \end{bmatrix} = 0 \quad \text{or} \quad \begin{pmatrix} W_{-\pi/a,-\pi/a} & V \\ V & W_{\pi/a,\pi/a} \end{pmatrix}\begin{bmatrix} C_{-\pi/a,-\pi/a} \\ C_{\pi/a} \end{bmatrix} = 0$$

A zero determinant of the C matrix means that

$$\det\begin{Bmatrix} \frac{\hbar^2}{2m_e}\left(\frac{2(-\pi)^2}{d^2}\right) - U & V \\ V & \frac{\hbar^2}{2m_e}\left(\frac{2(\pi)^2}{d^2}\right) - U \end{Bmatrix}$$

By defining $U_0 = 2\hbar\pi^2 / 2m_e d^2$, the determinant becomes

$$(U_0 - U_k + V)(U_0 - U_k) = U_k^2 - U_k(2U_0 + V) + U_0(U_0 + V) = 0$$

This is a simple quadratic equation in U_k which has the solution

$$U_k = U_0 + V/2 \pm V/2 \text{ ; i.e., } U_k = U_0 \text{ (n=1) or } U_0 + V \text{ (n=2)}$$

So the band gap at the corner point is simply equal to V !

5. Silicon statistical mechanics

(a) Density of states of single ellipsoid

For ellipsoidal constant energy surface oriented along *x* axis we have

$$U\text{-}U_C = \frac{\hbar^2}{2}\left[\frac{(k_X - k_{X0})^2}{m_l} + \frac{(k_Y - k_{Y0})^2}{m_t} + \frac{(k_Z - k_{Z0})^2}{m_t}\right] \qquad (*)$$

From geometry we know that an ellipsoid $\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1$ has a volume given by V = (4/3)πabc. This makes us rewrite (*) as

$$1 = \frac{(k_X - k_{X0})^2}{2m_l(\Delta U)/\hbar^2} + \frac{(k_Y - k_{Y0})^2}{2m_t(\Delta U)/\hbar^2} + \frac{(k_Z - k_{Z0})^2}{2m_t \Delta U/\hbar^2}$$

where $\Delta U \equiv U - U_C$. So a constant energy *U* surface defined about $\vec{k}_0 = (k_{X0}, k_{Y0}, k_{Z0})$ will have a volume given by

$$V = \frac{4}{3}\pi \frac{\sqrt{2m_l\Delta U}}{\hbar}\frac{\sqrt{2m_t\Delta U}}{\hbar}\frac{\sqrt{2m_t\Delta U}}{\hbar} = \frac{4\pi}{3}\frac{\sqrt{m_l m_t^2}(2\Delta U)^{3/2}}{\hbar^3}$$

and $$N(\vec{k}_0) \to N(U) = \frac{V}{4\pi^3}\frac{4\pi}{3}\frac{\sqrt{m_l m_t^2}(2\Delta U)^{3/2}}{\hbar^3} = \frac{V}{3\pi^2}\frac{\sqrt{m_l m_t^2}(2\Delta U)^{3/2}}{\hbar^3}$$

$$g_n(U) = \frac{dN}{dU} = \frac{V}{3\pi^2}\,\frac{3}{2}\,\frac{2^{3/2}\sqrt{m_l m_t^2}\,\Delta U^{1/2}}{\hbar^3} = \frac{V\sqrt{2}\sqrt{m_l m_t^2}\left(U\text{-}U_C\right)^{1/2}}{\pi^2\hbar^3}\ .$$

If we define: $g(U) \equiv \dfrac{\sqrt{2}V\left(m_d^*\right)^{3/2}\left(U - U_c\right)}{\pi^2\hbar^3}$,

then $\quad m_d^* = \left(m_l m_t^2\right)^{2/3} = \sqrt[3]{m_l m_t^2}$

and the specific density-of-states is

$$g'(U) = \frac{\sqrt{2}\sqrt{m_l m_t^2}\left(U - U_C\right)^{1/2}}{\pi^2\hbar^3}\ .$$

(b) Evaluation of key statistical mechanical properties for Si: At low temperature:
m_e=0.98 m_0, m_t=0.19 m_0, m_{lh}^*=0.16 m_0, m_{hh}^*=0.49 m_0, U_G=1.15 eV

a) so that density-of-states effective mass $\Rightarrow m_{d,c}^* = \sqrt[3]{m_e m_t^2} = 0.33\ m_0$

In valance band $m_d^* \Rightarrow m_{d,v}^* = \left[\left(m_{lh}^*\right)^{3/2} + \left(m_{hh}^*\right)^{3/2}\right]^{2/3} = 0.55\ \ m_0$

These numbers are only valid at low temperatures. At 300 K, data tables show $m_{d,c}^* \approx 0.36$ because band gap drops and masses rise with temperature. Also, $m_{d,v}^* \approx 0.81\ m_0$ because m_{lh}^* & m_{hh}^* both increase too.

b) effective density-of-states

$$N_C(T) = \frac{M}{4}\left(\frac{2m_{d,c}^* k_B T}{\pi\hbar^2}\right)^{3/2} = 3.21\times10^{25}\ m^3 = 3.22\times10^{19}\ cm^3 \quad @\ 300\text{ K}$$

$$N_V(T) = \frac{1}{4}\left(\frac{2m_{d,v}^* k_B T}{\pi\hbar^2}\right)^{3/2} = 1.83\times10^{25}\ m^3 = 1.83\times10^{19}\ cm^3 \quad @\ 300\text{ K}$$

$$n_i(T) = \left(N_C N_V\right)^{1/2} e^{-U_G/2k_B T} = 1.14\times10^{10}\,cm^3$$

for U_G = 1.11 eV @ 300 K

At 450 K, masses change again; so does U_G

$m_{d,c}^* \rightarrow 0.375 m_0$, $m_{d,v}^* \rightarrow 0.873 m_0$, U_G □ 1.07 eV

$N_C(T) \rightarrow$ 6.35x10^{19} cm^{-3}, $N_V(T) \rightarrow$ 3.76x10^{19} cm^{-3}, $n_i(T) \rightarrow$ 4.96x10^{13} cm^{-3}