SOLUTION to Exam May 28, 2009

Problem 1

a) The primitive vectors are: **a**=½a(-1,1,1), **b**=½a(1,-1,1), **c**=½a(1,1,-1)
The angle between vectors: **a**· **b**= -½√3a½√3a cosθ = ¼a^2.
Therefore: cosθ =-1/3 og θ = 109.5°.
The volume of the primitive cell is a^3/2 (2 atoms in the FCC cell).
The primitive reciprocal lattice vectors for the FCC lattice:

$$a^* = \frac{2\pi \boldsymbol{b}\times\boldsymbol{c}}{\boldsymbol{a}\cdot(\boldsymbol{b}\times\boldsymbol{c})} = \frac{4\pi}{a^3}a^2(\hat{x}-\hat{y}+\hat{z})\times(\hat{x}+\hat{y}-\hat{z}) = \frac{4\pi}{a}(\hat{z}+\hat{y}+\hat{z}+\hat{x}+\hat{y}-\hat{x}) = \frac{2\pi}{a}(0,1,1)$$

$$b^* = \frac{2\pi \boldsymbol{c}\times\boldsymbol{a}}{\boldsymbol{a}\cdot(\boldsymbol{b}\times\boldsymbol{c})} = \frac{4\pi}{a^3}a^2(\hat{x}+\hat{y}-\hat{z})\times(-\hat{x}+\hat{y}+\hat{z}) = \frac{4\pi}{a}(\hat{z}-\hat{y}+\hat{z}+\hat{x}+\hat{y}+\hat{x}) = \frac{2\pi}{a}(1,0,1)$$

$$c^* = \frac{2\pi \boldsymbol{a}\times\boldsymbol{b}}{\boldsymbol{a}\cdot(\boldsymbol{b}\times\boldsymbol{c})} = \frac{4\pi}{a^3}a^2(-\hat{x}+\hat{y}+\hat{z})\times(\hat{x}-\hat{y}+\hat{z}) = \frac{4\pi}{a}(\hat{z}+\hat{y}-\hat{z}+\hat{x}+\hat{y}+\hat{x}) = \frac{2\pi}{a}(1,1,0)$$

This shows that the reciprocal lattice of the BCC structure is the FCC lattice.

b) The tetrahedron has 24 GEP. Therefore there are 24 symmetry elements in the point group:

$$1, 3\times\bar{4}^1, 3\times\bar{4}^2, 3\times\bar{4}^3, 4\times 3^1, 4\times 3^2, 6\times m$$

identity, four-fold inversion axes, three-fold rotation axes, mirror planes

c) The Laue condition for x-ray diffraction $e^{i\boldsymbol{K}\cdot\boldsymbol{R}_{uvw}} = 1$ where $\boldsymbol{K}$ is the scattering vector and $\boldsymbol{R}_{uvw}$ is a real space lattice vector. This means that the scattering vector $\boldsymbol{K}$ must be a reciprocal lattice vector.

The extinction rules (norsk: utslokkingregler) for the FCC structure may be found by noting that this structure may be viewed as a simple cubic structure with a basis (0,0,0) , (½,½,0), (½,0,½) and (0,½,½). The structure factor (or scattering amplitude) is then:

$$F_{hkl} = f(1 + e^{\pi i(h+k)} + e^{\pi i(h+l)} + e^{\pi i(k+l)})$$

which becomes zero for $h+k = 2n+1$ or $h+l = 2n+1$ or $k+l = 2n+1$ is an odd number.

d) $A = \sum_{i\neq j}\frac{\pm 1}{a_{ij}^n}$ = the Madelung constant,

β = constant describing the strength of the repulsive part of the potential, n = integer describing the range of the repulsive part of the potential

$b = \sum_{i\neq j}\frac{1}{a_{ij}^n}$ = is a sum over atoms (repulsive part)

q = the charge on the ions (+ or -)
R = nearest neighbor separation
R_0 defines the equilibrium distance, and is given by: $\frac{\partial U}{\partial R} = 0 \Rightarrow R_0^{n-1} = \frac{4\pi\varepsilon_0 n\beta b}{Aq^2}$

The volume of the solid is given by: $V = 2NR^3$, where 2N = number of ions in the NaCl structure.

To find the Bulk modulus we have to differentiate U with respect to the volume V twice:

$$\frac{\partial U}{\partial V} = \left(\frac{\partial U}{\partial R}\right)\left(\frac{\partial R}{\partial V}\right) \Rightarrow \frac{\partial^2 U}{\partial V^2} = \left(\frac{\partial U}{\partial R}\right)\left(\frac{\partial^2 R}{\partial V^2}\right) + \left(\frac{\partial^2 U}{\partial R^2}\right)\left(\frac{\partial R}{\partial V}\right)^2$$

The first term on the right hand side disappears at the equilibrium position R_0.
Furthermore:

$$\left(\frac{\partial R}{\partial V}\right)_0^2 = \frac{1}{36N^2R_0^4} \Rightarrow \left(\frac{\partial^2 U}{\partial V^2}\right)_0 = \frac{1}{36N^2R_0^4}\left(\frac{\partial^2 U}{\partial R^2}\right)_0$$

Where:

$$\frac{\partial U}{\partial R} = N\left(\frac{-\beta bn}{R^{n+1}} + \frac{Aq^2}{4\pi\varepsilon_0 R^2}\right) \Rightarrow \frac{\partial^2 U}{\partial R^2} = N\left(\frac{\beta bn(n+1)}{R^{n+2}} - \frac{2Aq^2}{R^3}\right)$$

The Bulk modulus is then:

$$B = V\left(\frac{\partial^2 U}{\partial V^2}\right)_0 = \frac{1}{18NR_0}\left(\frac{\partial^2 U}{\partial R^2}\right)_0 = \frac{1}{18R_0}\left(\frac{\beta bn(n+1)}{R_0^{n+2}} - \frac{2Aq^2}{R_0^3}\right)$$

$$B = \frac{1}{18R_0}\left(\frac{Aq^2(n+1)}{4\pi\varepsilon_0 R_0^3} - \frac{2Aq^2}{R_0^3}\right) = \frac{Aq^2}{72\pi\varepsilon_0 R_0^4}(n+1-2)$$

$$\boxed{B = \frac{Aq^2(n-1)}{72\pi\varepsilon_0 R_0^4}}$$

Problem 2

(a)

(i) 3D free electron density of states:

$$e^{ikx} = e^{ik(x+L)} \Rightarrow kL = n2\pi \Rightarrow k = n\frac{2\pi}{L} \qquad \text{periodic boundary conditions}$$

$$\left(\frac{L}{2\pi}\right)^3 \qquad \text{is the number of states per unit volume in k-space}$$

$$g(k)dk = 2\cdot\left(\frac{L}{2\pi}\right)^3\cdot 4\pi k^2\cdot dk = g(E)dE$$

$$E = \frac{\hbar^2k^2}{2m} \Rightarrow g(E) = \frac{g(k)}{\frac{dE}{dk}} = \frac{mL^3}{\hbar^2\pi^2}k = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}E^{\frac{1}{2}}$$

(ii) Fermi-energy:

$$N = \int_0^{E_F} g(E)dE = \frac{V}{3\pi^2}\left(\frac{2mE_F}{\hbar^2}\right) \Rightarrow E_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}}$$

(iii) Average electron energy at $T = 0\ K$:

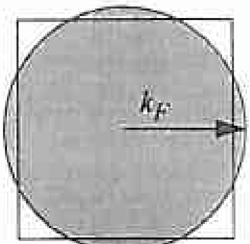
$$\langle E\rangle = \int_0^{E_F} Eg(E)dE = \frac{V}{3\pi^2}\left(\frac{2mE_F}{\hbar^2}\right)^{\frac{3}{2}} \cdot \frac{3}{2} \cdot \frac{2}{5}E_F = \frac{3}{5}NE_F$$

(b) Fermi wave-vector in 2D (N_c is the number of electrons in unit cell):

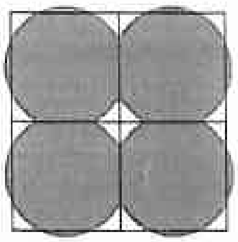
$$g'(E) = \frac{ma^2}{\hbar^2\pi} \qquad \text{2D–density of states (per unit cell)}$$

$$N_c = \int_0^{E_F} g'(E)dE = \frac{ma^2}{\hbar^2\pi}E_F \Rightarrow k_F = \frac{\sqrt{2mE_F}}{\hbar} = \frac{\pi}{a}\sqrt{\frac{2N_c}{\pi}} = \frac{\pi}{a}\cdot 1{,}13 \qquad (N_c = 2)$$

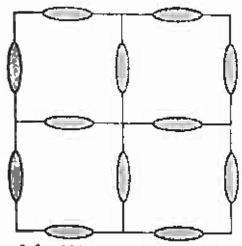
Fermi surface:



Fermi wave vector k_F



1st Brillouin zone
Fermi surface (hole-pockets)



2nd brillouin zone
Fermi surface (electron-pockets)

(Repeated zone scheme)

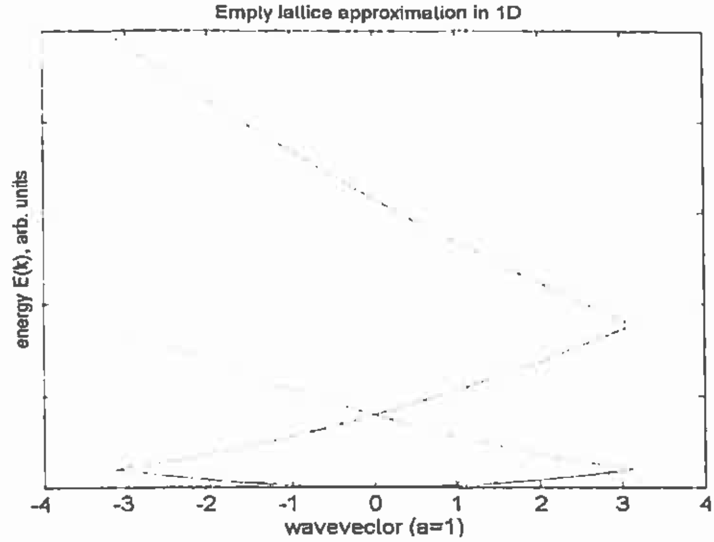
The Fermi surface does not extend into the 3rd Brillouin zone (2 electrons in unit cell).
The 3rd BZ is the hatched areas in the figure in problem 3.

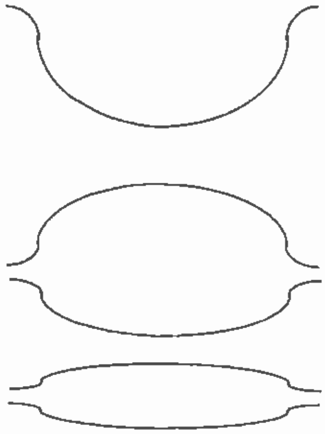
(c) Empty-lattice approximation in 1D.
The "empty lattice" approximation describes "free" electrons that are confined to a periodic lattice.
The wavevector of the electron is determined moduli a reciprocal lattice vector.
The electronic band structure *E(k)* for a one-dimensional system of lattice spacing a is given by:

$$E(k) = \frac{\hbar^2}{2m}(k + G)^2$$

$$where \qquad G = \pm n\frac{2\pi}{a}$$

The lowest energybands:





NFE model (qualitative changes)

(d) Form the algebraic S-eq.

$$\left(\frac{\hbar^2 k^2}{2m} - E\right)C_k + \sum_G V_G C_{k-G} = 0$$

we get the following set of equations, using $\lambda = \hbar^2\left(\frac{G}{2}\right)^2/2m$

$$(\lambda - E)C_{\frac{G}{2}} + V_G C_{\frac{-G}{2}} = 0 \qquad and \qquad (\lambda - E)C_{\frac{-G}{2}} + V_{-G} C_{\frac{G}{2}} = 0$$

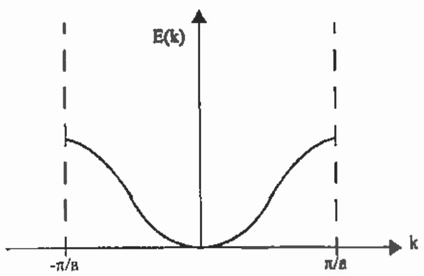
These equations have solution if the determinand vanishes

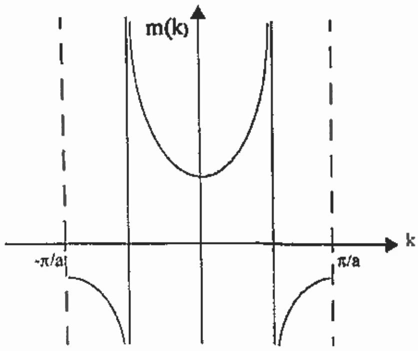
$$\begin{bmatrix} \lambda - E & V_G \\ V_{-G} & \lambda - E \end{bmatrix} = 0 \Rightarrow (\lambda - E)^2 - |V_G|^2 = 0 \Rightarrow E = \lambda \pm |V_G| \Rightarrow \Delta E = 2|V_G| = 0{,}2eV$$

The bandgap ΔE = 0.2 eV.

Problem 3

a) Effective electron mass is inversely proportional to the curvature of the electron band.





b) The concentration n of electrons in the conduction band of an intrinsic semiconductor at T = 300 K, a value of the energy gap of 1.2 eV (i.e. E_c-μ=0.6 eV), and an effective electron mass of 50% of the mass of a free electron:

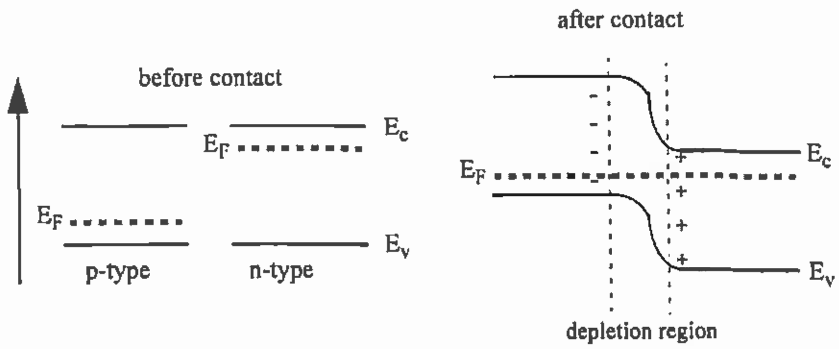
$$n = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{\frac{3}{2}} e^{-(E_c-\mu)/k_B T} = 7.5\cdot 10^{14}\ \mathrm{m}^{-3} = p$$

c) The position of the donor level relative to the bottom of the conduction band for the semiconductor as shown in the figure, when the effective mass of the electron $m_e^* = 0.1\ m_e$ and the dielectric constant of the semiconductor $\varepsilon = 10\ \varepsilon_0$ may be found by using the exprcssion for the Rydberg constant. The radius of the orbital may be found from the expression of the Bohr radius:

$$E_n = -R_0/n^2 \qquad where \qquad R_0 = \frac{e^4 m_e}{32\pi^2\varepsilon_0^2\hbar^2} = 13{,}6eV$$

$$E_d = R_0 \cdot \frac{m_e^*}{m_e} \cdot \left(\frac{\varepsilon_0}{\varepsilon}\right)^2 = \frac{R_0}{1000} = 13{,}6meV$$

$$r_d = \left(\frac{m_e}{m_e^*}\right)\varepsilon a_0 \approx 5{,}3nm$$



d) The potential across the junction is caused by diffusion of electrons from the n-side to the p-side and diffusion of holes from the p-side to the n-side. Equilibrium is established between the recombination currents (electrons recombinates with holes) and generating currents (thermal excitation of electrons to the conduction band) to prevent build up of charges. The electric field across the depletion layer removed electrons and holes, and therefore the number of charge carriers is low and the resistance is high.