

SOLUTION to Exam Dec. 16, 2008

Problem 1

- a) The primitive vectors are: $\mathbf{a} = \frac{1}{2}a(-1, 1, 1)$, $\mathbf{b} = \frac{1}{2}a(1, -1, 1)$, $\mathbf{c} = \frac{1}{2}a(1, 1, -1)$

The angle between vectors: $\mathbf{a} \cdot \mathbf{b} = -\frac{1}{2}\sqrt{3}a\frac{1}{2}\sqrt{3}a \cos\theta = \frac{1}{4}a^2$.

Therefore: $\cos\theta = -1/3$ og $\theta = 109.5^\circ$.

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:

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

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

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

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

- b) By studying the FCC structure we find: 4 3-fold and 3 4-fold rotation axes.

Also, 9 mirror planes may be identified.

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

The extinction rules (norsk: utsløkkingsregler) for the BCC structure may be found by noting that this structure may be viewed as a simple cubic structure with a basis (0,0,0) and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. The structure factor (or scattering amplitude) is then:

$$F_{hkl} = f \left(1 + e^{2\pi i \left(\frac{1}{2}h + \frac{1}{2}k + \frac{1}{2}l \right)} \right) = f(1 + e^{\pi i(h+k+l)})$$

which becomes zero for $h+k+l = 2n+1 = \text{an odd number}$.

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

$\beta = \text{constant describing the strength of the repulsive part of the potential, } n = \text{integer describing the range of the repulsive part of the potential}$

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

$q = \text{the charge on the ions (+ or -)}$

$R = \text{nearest neighbor separation}$

R_0 defines the equilibrium distance, and is given by: $\frac{\partial U}{\partial R} = 0 \Rightarrow R_0^{n-1} = \frac{4\pi\epsilon_0 n \beta b}{A q^2}$

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

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:

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

Where:

$$\frac{\partial U}{\partial R} = N \left(\frac{-\beta b n}{R^{n+1}} + \frac{A q^2}{4\pi \epsilon_0 R^2} \right) \Rightarrow \frac{\partial^2 U}{\partial R^2} = N \left(\frac{\beta b n(n+1)}{R^{n+2}} - \frac{2A q^2}{R^3} \right)$$

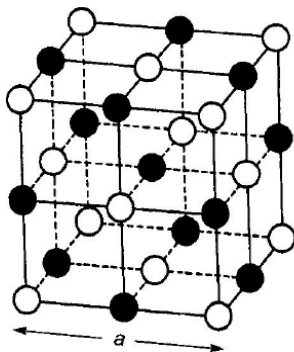
The Bulk modulus is then:

$$B = V \left(\frac{\partial^2 U}{\partial V^2} \right)_0 = \frac{1}{18N R_0} \left(\frac{\partial^2 U}{\partial R^2} \right)_0 = \frac{1}{18R_0} \left(\frac{\beta b n(n+1)}{R_0^{n+2}} - \frac{2A q^2}{R_0^3} \right)$$

$$B = \frac{1}{18R_0} \left(\frac{A q^2 (n+1)}{4\pi \epsilon_0 R_0^3} - \frac{2A q^2}{R_0^3} \right) = \frac{A q^2}{72\pi \epsilon_0 R_0^4} (n+1-2)$$

$$B = \frac{A q^2 (n-1)}{72\pi \epsilon_0 R_0^4}$$

Contribution to the Madelung constant from one unit cell.



$$\text{The Madelung constant } A = \sum_{i \neq j} \frac{\pm 1}{a_{ij}}$$

where + means ions of opposite polarity
and - means ions of same polarity

a_{ij} is the distance between ions i and j in units
of R (nearest neighbor distance)

Consider the central atom (e.g. Na).

Nearest neighbors (Cl) on face centers (0.5 of each atom inside cell) : 6 at distance R

Next nearest neighbors (Na) on edges (0.25 of each atom inside cell): 12 at distance $\sqrt{2}R$

Next nearest neighbors (Cl) on corners (0.125 of each atom inside cell): 8 at distance $\sqrt{3}R$

$$\text{Therefore } A = \frac{1}{2} \cdot 6 \cdot \frac{1}{1} - \frac{1}{4} \cdot 12 \cdot \frac{1}{\sqrt{2}} + \frac{1}{8} \cdot 8 \cdot \frac{1}{\sqrt{3}} = 1.46$$

($A = 1.75$ if the sum is over all ions in the crystal)

Problem 2

(a)

(i) 3D free electron density of states:

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

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

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

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

(ii) Fermi-energy:

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

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

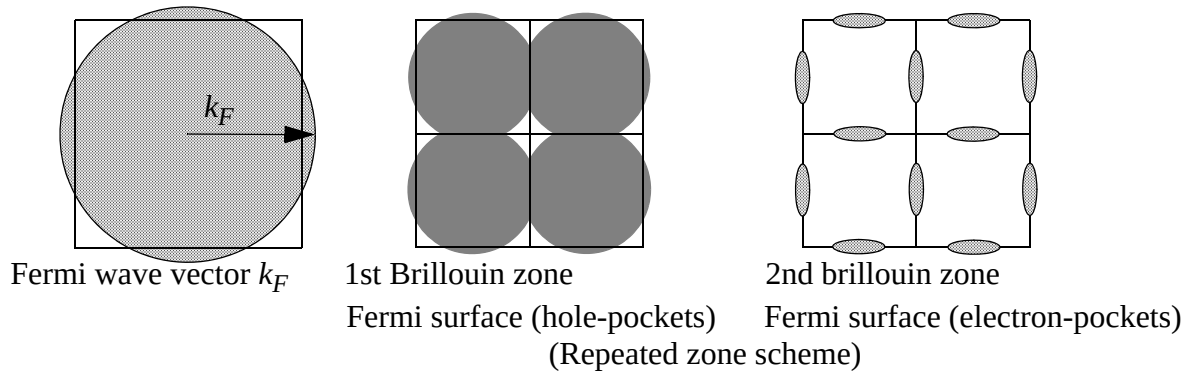
$$\langle E \rangle = \int_0^{E_F} E g(E)dE = \frac{V}{3\pi^2} \left(\frac{2mE_F}{\hbar^2}\right)^{\frac{3}{2}} \cdot \frac{3}{2} \cdot \frac{2}{5} E_F = \frac{3}{5} N E_F$$

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

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

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

Fermi surface:



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.

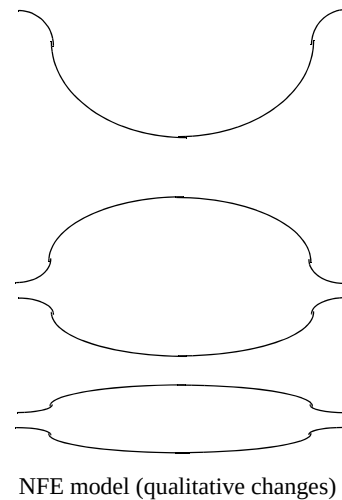
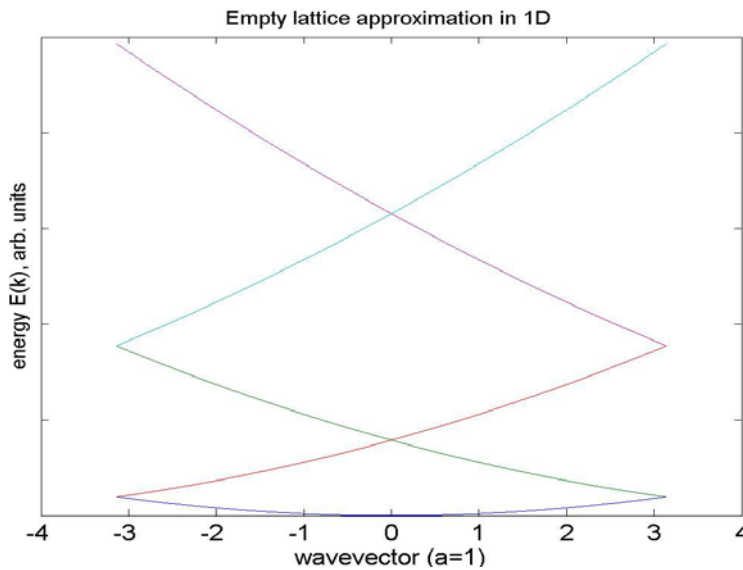
The “empty lattice” approximation describes “free” electrons that are confined to a periodic lattice. The wavevector of the electron is determined modulo a reciprocal lattice vector.

The electronic band structure $E(k)$ for a one-dimensional system of lattice spacing a is given by:

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

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

The lowest energy bands:



(d) Phonon annihilation process (two TA phonons recombine to one LA phonon):

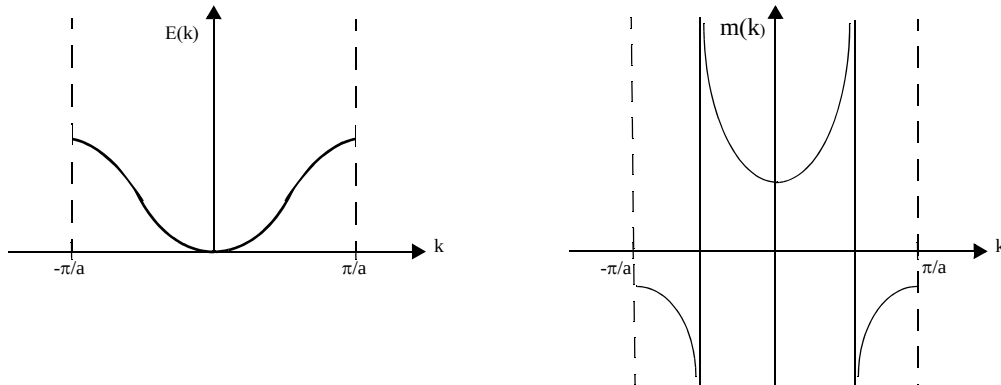
$$k_3 = k_1 + k_2 + G = \frac{2\pi}{3a} + \frac{2\pi}{3a} + G = \frac{4\pi}{3a} - \frac{2\pi}{a} = -\frac{2\pi}{3a} \quad \text{inside 1st Brillouin zone}$$

$$\omega_3 = \omega_1 + \omega_2 = \omega_0 \left| \sin \frac{\pi}{3} \right| + \omega_0 \left| \sin \frac{\pi}{3} \right| = 2\sqrt{3} = 2\omega_0 \left| \sin \left(-\frac{\pi}{3} \right) \right|$$

Both crystal momentum and energy conservation laws are satisfied in this process.

Problem 3

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



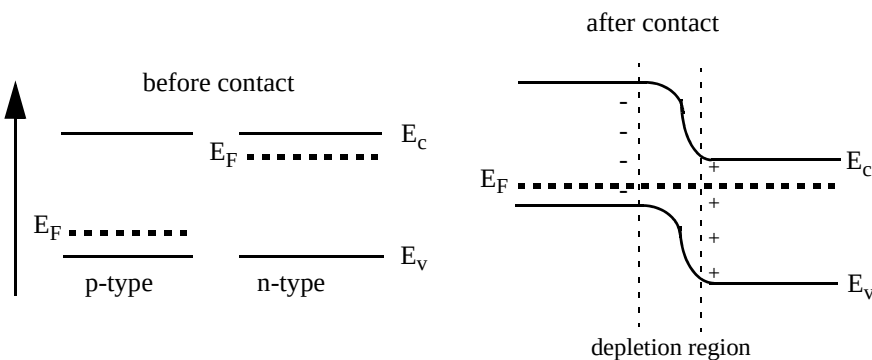
- b) The concentration n of electrons in the conduction band of an intrinsic semiconductor at $T = 300$ K, a value of the energy gap of 1.2 eV (i.e. $E_c - \mu = 0.6$ eV), and an effective electron mass of 50% of the mass of a free electron:

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

- 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 $\epsilon = 10 \epsilon_0$ may be found by using the expression for the Rydberg constant:

$$E_n = -R_0/n^2 \quad \text{where} \quad R_0 = \frac{e^4 m_e}{32\pi^2 \epsilon_0^2 \hbar^2} = 13.6 \text{ eV}$$

$$E_d = R_0 \cdot \frac{m_e^*}{m_e} \cdot \left(\frac{\epsilon_0}{\epsilon} \right)^2 = \frac{R_0}{1000} = 13.6 \text{ meV}$$



- 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 recombines 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.