

### SOLUTION Exam June 10, 2010

#### Problem 1

- a) The primitive translation vectors of a hexagonal lattice may be written (other choices are also possible and are equally valid):

$$\mathbf{a} = (\sqrt{3}a/2)\hat{x} + (a/2)\hat{y} \quad \mathbf{b} = -(\sqrt{3}a/2)\hat{x} + (a/2)\hat{y} \quad \mathbf{c} = c\hat{z}$$

The angles between the vectors are given by:

$$\mathbf{a} \cdot \mathbf{b} = abc \cos \theta \Rightarrow \cos \theta = \left(-\frac{3}{4} + \frac{1}{4}\right) / \left(\frac{3}{4} + \frac{1}{4}\right) = -\frac{1}{2} \Rightarrow \theta = 120^\circ$$

The volume is given by:

$$\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = ((\sqrt{3}a/2)\hat{x} + (a/2)\hat{y}) \cdot \left(\sqrt{3}\frac{ac}{2}\hat{y} + \frac{ac}{2}\hat{x}\right) = \frac{\sqrt{3}a^2c}{2}$$

The reciprocal lattice vectors becomes

$$\mathbf{a}^* = \frac{2\pi\mathbf{b} \times \mathbf{c}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})} = \frac{4\pi}{\sqrt{3}a^2c} \left(-\frac{\sqrt{3}a}{2}\hat{x} + \frac{a}{2}\hat{y}\right) \times c\hat{z} = \frac{4\pi}{\sqrt{3}a^2c} \left(\frac{ac}{2}\hat{x} + \frac{\sqrt{3}ac}{2}\hat{y}\right) = \frac{2\pi}{\sqrt{3}a}\hat{x} + \frac{2\pi}{a}\hat{y}$$

$$\mathbf{b}^* = \frac{2\pi\mathbf{c} \times \mathbf{a}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})} = \frac{4\pi}{\sqrt{3}a^2c} c\hat{z} \times \left(\frac{\sqrt{3}a}{2}\hat{x} + \frac{a}{2}\hat{y}\right) = \frac{4\pi}{\sqrt{3}a^2c} \left(-\frac{ac}{2}\hat{x} + \frac{\sqrt{3}ac}{2}\hat{y}\right) = -\frac{2\pi}{\sqrt{3}a}\hat{x} + \frac{2\pi}{a}\hat{y}$$

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

- b) There are 6 GEP in the NH<sub>3</sub> molecule.

Therefore there are 6 symmetry elements in the point group: E, C<sub>3</sub>, C<sub>3</sub><sup>2</sup>, 3σ<sub>v</sub> identity, three-fold rotation axes, mirror planes

- 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: utslokkingregler) 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), (1/2,1/2,1/2).

The structure factor (or scattering amplitude) is then:

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

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

- d) The common types of bonding in a solid are:

- (1) ionic bonding, centrosymmetric, long ranged
- (2) metallic bonding, centrosymmetric, long ranged
- (3) covalent bonding, directional, short ranged
- (4) van der Waals bonding, weak, centrosymmetric, short ranged
- (5) hydrogen bonding, short ranged, crystalline ice, biological systems

**Problem 2**

(a) We consider the Bloch function  $\psi(x) = e^{ikx} u_k(x)$  and use periodic boundary conditions to realize that  $\psi(x + Na) = e^{ik(x+Na)} u_k(x+Na) = e^{ikNa} \psi(x) = \psi(x)$  since  $u_k$  is periodic.

Therefore a requirement is that  $e^{ikNa} = 1$ , and we get

$$k = n \frac{2\pi}{Na} = 0, \pm \frac{2\pi}{Na}, \pm 2 \frac{2\pi}{Na}, \dots, \pm \frac{\pi}{a} = \frac{2\pi(N/2)}{Na}$$

since  $k = +\pi/a$  and  $k = -\pi/a$  are connected by a reciprocal lattice vector and represent the same state, we find that there are  $N$  distinct states.

(b)

(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:

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

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

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

(c) Empty-lattice approximation in 1D.

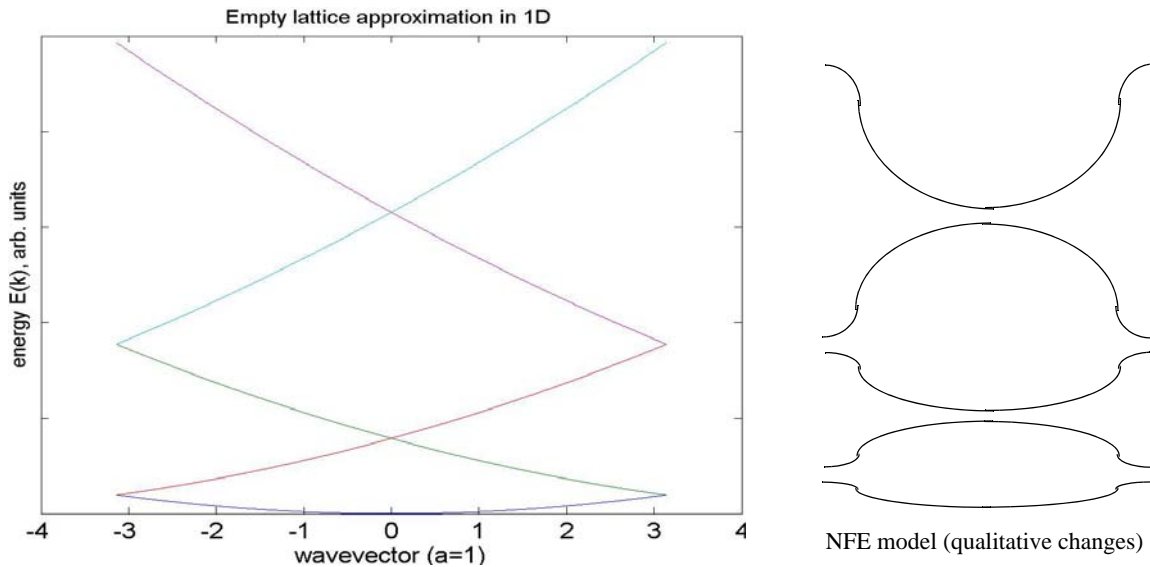
The “empty lattice” approximation describes “free” electrons that are confined to a periodic lattice. The wavevector of the electron is determined modulo a reciprocal lattice vector.

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

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

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

The lowest energybands:



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

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

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

### Problem 3

- a) The concentration  $n$  of electrons in the conduction band of an intrinsic semiconductor at  $T = 300$  K, a value of the energy gap of 1.42 eV, and an effective masses  $m_e^* = 0.07m_e$ ,  $m_h^* = 0.05m_e$ :

$$n = \sqrt{n \cdot p} = 2 \left( \frac{2\pi k_B T}{h^2} \right)^{\frac{3}{2}} (m_e^* m_h^*)^{\frac{3}{4}} e^{\frac{3}{4} \frac{-E_{gap}}{2k_B T}} = 4.3 \cdot 10^{11} \text{ m}^{-3} = p$$

The chemical potential  $\mu$  is found by  $n = p$  which gives:

$$\mu = \frac{E_c + E_v}{2} + \frac{3}{4} k_B T \ln \left( \frac{m_h^*}{m_e^*} \right)$$

- b) Mobility

$$\sigma = ne\mu_e + pe\mu_h \quad \text{and} \quad n \propto e^{-E_{gap}/2k_B T}$$

$$\text{Numerical value } \sigma = 3.2 \cdot 10^{-8} \Omega^{-1} \text{m}^{-1}$$

The conductivity increases with temperature as  $e^{-E_{gap}/2k_B T}$

- 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 expression for the Rydberg constant. The radius of the orbital may be found from the expression of the Bohr radius:

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

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

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

- d) Negative effective mass.

A negative mass would be unphysical for a free electron. However, for an electron in a solid the motion is linked to the lattice. Let us consider an electron in a band with wavevector  $k$  near the zone boundary. An increase in  $k$  by an electric field takes the electron closer to the condition of Bragg-reflection ( $k=\pi/a$ ), therefore momentum transfer from the electron to the lattice following elastic back scattering is greater than the increase in  $k$  by the electric field. Thus the effective mass is negative. Therefore negative mass effects are only significant for nearly full bands.