

NORGES TEKNISK-
NATURVITENSKAPELIGE UNIVERSITET
INSTITUTT FOR FYSIKK

Fagleg kontakt under eksamen:
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Eksamen i Emne TFY4220 Faste Stoffers Fysikk

Tirsdag 16. desember 2008
Tid: kl 09.00-13.00

Hjelpemiddel: Alternativ C

Godkjend lommekalkulator (approved pocket calculator)

K. Rottman: Matematisk formelsamling (alle språkutgaver)

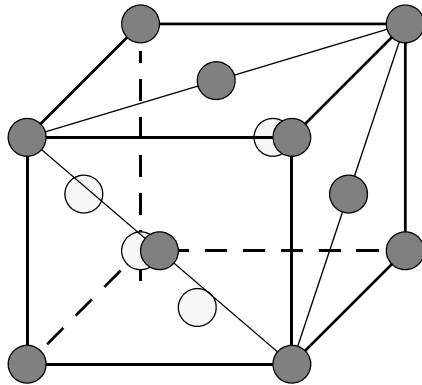
Engelsk ordbok (English dictionary) (alle språk)

VEDLEGG (Appendix):

Vedlegg: formelark (constants and formulas)

Problem 1

- (a) Derive the primitive lattice vectors for the BCC unit cell in terms of the lattice parameter a .
 Find the angles between the primitive lattice vectors.
 What is the volume of the primitive cell?
 Find the reciprocal lattice vectors. What is the lattice structure in reciprocal space?



- (b) The figure above shows the FCC structure.
 How many 4-fold and 3-fold rotation axis describe this structure?
 How many mirror planes are contained in the structure?
- (c) Formulate the Laue condition for x-ray diffraction and define the involved quantities.
 Derive the extinction rules (norsk: utslokkingsregler) for the BCC structure.
- (d) The total lattice energy for an ionic solid may be described by the Born-Landé equation:

$$U = N \left(\frac{\beta b}{R^n} - \frac{Aq^2}{4\pi\epsilon_0 R} \right)$$

Define the quantities in the above equation.

The bulk modulus B is a measure of the stiffness of the ionic solid, and is given by:

$$B = V \left(\frac{\partial^2 U}{\partial V^2} \right)_0$$

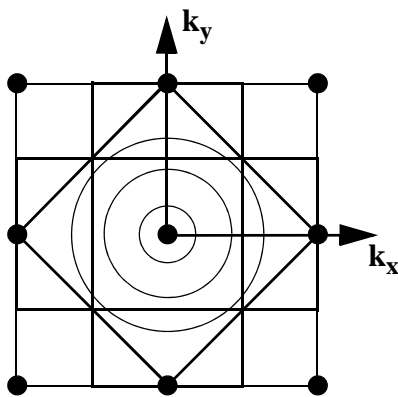
where the subscript 0 refers to the equilibrium distance R_0 between atoms in the solid.

Find an expression for the bulk modulus B expressed by R_0 , A , q and n .

Define the Madelung constant and calculate the contribution to the Madelung constant from one unit cell for NaCl.

(Tip: start with the central atom in the unit cell and consider the nearest, next nearest, and third nearest neighbors.)

Problem 2



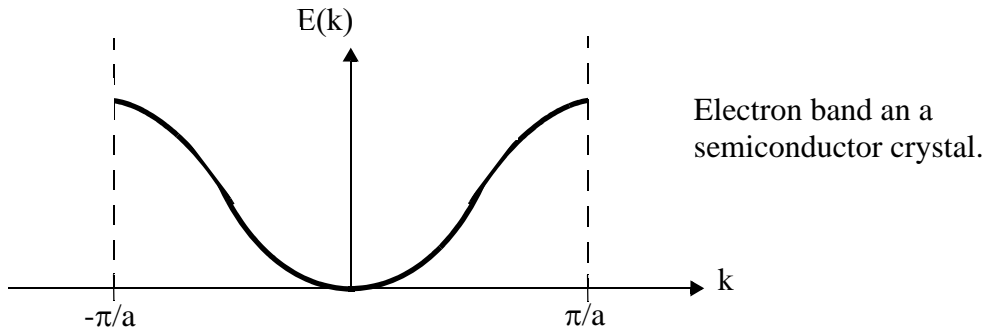
The figure shows a two dimensional reciprocal lattice. The circles represent constant energy contours in the free electron model.

- (a) Derive the 3D density of states $g(E)$, find the Fermi energy in terms of the electron density n , and find the average electron energy at $T = 0$ K in the free electron model.
- (b) Find the Fermi wave vector k_F for the 2D system that corresponds to the figure above, in the case of 2 electrons per unit cell. Use this to sketch qualitatively the Fermi surface in the 1st and 2nd Brillouin zones in the repeated zone scheme. Does the Fermi surface exist in the 3rd Brillouin zone? Explain.
- (c) Compute the three lowest energy bands in the empty-lattice approximation in one dimension. Plot these bands in an $E(k)$ versus k diagram, using the reduced-zone scheme. Show qualitatively how these bands are modified in the NFE (nearly free electron) model.
- (d) Consider a phonon annihilation process in which two transverse acoustic phonons combine to one longitudinal acoustic phonon. Assume that the phonon wave vectors are all parallel. The dispersion relations for transverse and longitudinal acoustic phonons are:

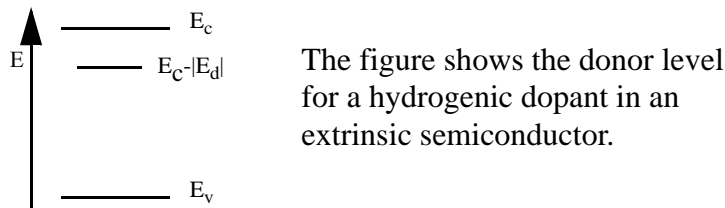
$$\omega_{TA} = \omega_0 \left| \sin\left(\frac{ka}{2}\right) \right| \quad \text{and} \quad \omega_{LA} = 2\omega_0 \left| \sin\left(\frac{ka}{2}\right) \right|$$

Determine if this is an allowed process for acoustic wave vectors $k_1 = k_2 = \frac{2\pi}{3a}$. Explain your reasoning!

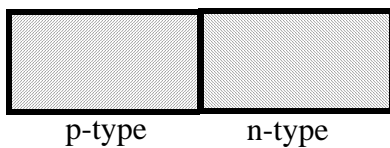
Problem 3



- (a) Sketch qualitatively the effective electron mass corresponding to the electron band shown in the figure above. Please explain your reasoning.
- (b) Find the concentration n of electrons in the conduction band for an intrinsic semiconductor when $T = 300\text{ K}$ and the value of the energy gap is $E_g = 1.2\text{ eV}$. Assume that the effective mass of the electrons is 50% of the mass of a free electron. Find the concentration p of holes in the valence band.



- (c) Find the position of the donor level relative to the bottom of the conduction band for the semiconductor as shown in the figure above, when the effective mass of the electron $m_e^* = 0.1 m_e$ and the dielectric constant of the semiconductor $\epsilon = 10 \epsilon_0$.



The figure shows a semiconductor pn-junction.

- (d) Draw the energy diagram for p-type and n-type semiconductor before they are contacted. Also draw the energy diagram after they are contacted. Show the Fermi level. What is the origin of the potential difference across the junction? Give a brief qualitatively description of the resistance and number of charge carriers in the depletion region.

Vedlegg (Appendix): Some constants and expressions that may or may not be of use.

$$\begin{array}{lll} k_B = 1.38 \cdot 10^{-23} \text{ J/K} & e = 1.6 \cdot 10^{-19} \text{ C} & \epsilon_0 = 8.85 \cdot 10^{-12} \text{ s}^4 \text{ A}^2 \text{ kg}^{-1} \text{ m}^{-3} \\ h = 6.63 \cdot 10^{-34} \text{ Js} & m_e = 9.1 \cdot 10^{-31} \text{ kg} & c = 3.0 \cdot 10^8 \text{ m/s} \\ \hbar = h/2\pi = 1.05 \cdot 10^{-34} \text{ Js} & R_0 = 13.6 \text{ eV} & \end{array}$$

$$\left. \begin{array}{l} \frac{1}{1-x} \approx 1 + x + x^2 \dots \\ \sin x \approx x - \frac{1}{3!} x^3 \dots \\ \sqrt{1+x} \approx 1 + \frac{x}{2} + \dots \end{array} \right\} \text{ for } x \ll 1$$

$$n(\omega) = \frac{1}{e^{\hbar\omega/k_B T} - 1} \quad \text{Planck distribution law for phonons} \\ \text{(average phonon occupation number)}$$

$$\omega(k) = 2 \sqrt{\frac{K}{M}} \left| \sin \frac{ka}{2} \right| \quad \text{phonon dispersion relation}$$

$$g(E) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} E^{1/2} \quad \text{3D free-electron density of states}$$

$$g(E) = \frac{mL^2}{\hbar^2 \pi} \quad \text{2D free-electron density of states}$$

$$E_n = -R_0/n^2 \quad \text{energy levels of the hydrogen atom}$$

$$R_0 = \frac{e^4 m_e}{32\pi^2 \epsilon_0^2 \hbar^2} \quad \text{the Rydberg constant}$$

$$f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1} \quad \text{Fermi-Dirac distribution function} \\ \text{(Fermi-function)}$$

$$n = 2 \left(\frac{2\pi m_e^* k_B T}{\hbar^2} \right)^{3/2} e^{-(E_c - \mu)/k_B T} = N_c e^{-(E_c - \mu)/k_B T}$$

$$p = 2 \left(\frac{2\pi m_h^* k_B T}{\hbar^2} \right)^{3/2} e^{(E_v - \mu)/k_B T} = N_v e^{(E_v - \mu)/k_B T}$$