NTNU
Kunnskap for en bedre verden

Department of physics

Examination paper for TFY4220 Solid State Physics

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Examination date:	**__ August 2017**
Examination time (from - to):	**09:00 – 13:00**

Permitted examination support material:

C: *Simple calculator*
K. Rottmann: Matematisk Formelsamling
Barnett & Cronin: Mathematical Formulae

Other information

All the subtasks a), b), … are given equal weight.

Language:	**English**
Number of pages (front page excluded):	**3**
Number of pages enclosed ("vedlegg"):	**1**

Informasjon om trykking av eksamensoppgave
Originalen er:

1-sidig ☐ **2-sidig** ☐

sort/kvit ☐ **farger** ☐

Skal ha flervalgsskjema ☐

Checked by:

Date Signature

NB! Attachment.

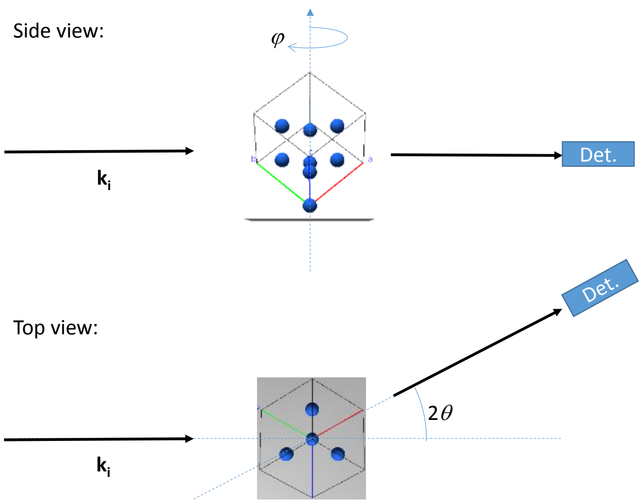
Problem 1

Silicon (Si) has diamond structure, which is cubic with a = 5.43 Å.

a) What is meant by “extinct” or “systematically absent” diffraction peaks?
The reflections for the diamond structure are non-extinct if:
- h,k,l all odd, *or*
- h,k,l all even and $h+k+l = 4n$ (where n is an integer)

What are the three lowest order non-extinct reflections of Si?

b) Derive Bragg’s law. At what scattering angle 2θ can the $\{220\}$ reflections be observed? Assume that monochromatic X-ray radiation with a wavelength of 1.5418 Å is used.



Assume now that a silicon single crystal is oriented with its $[111]$ axis parallel to the 2θ rotation axis of the detector, as shown in the figure above.

c) We now assume that the detector position is fixed in the horizontal plane, normal to $[111]$, at the scattering angle 2θ for the $\{220\}$ reflections. The sample crystal is rotated about the axis φ from 0° to 360°, while the intensity $I(\varphi)$ is recorded with a counting detector. Sketch what the intensity distribution $I(\varphi)$ will look like, and which reflections that will be observed!
Hint: $2\bar{2}0$ is one of the reflections that will be seen.

d) State and explain Bloch’s theorem. Comment shortly on the choice of boundary conditions.

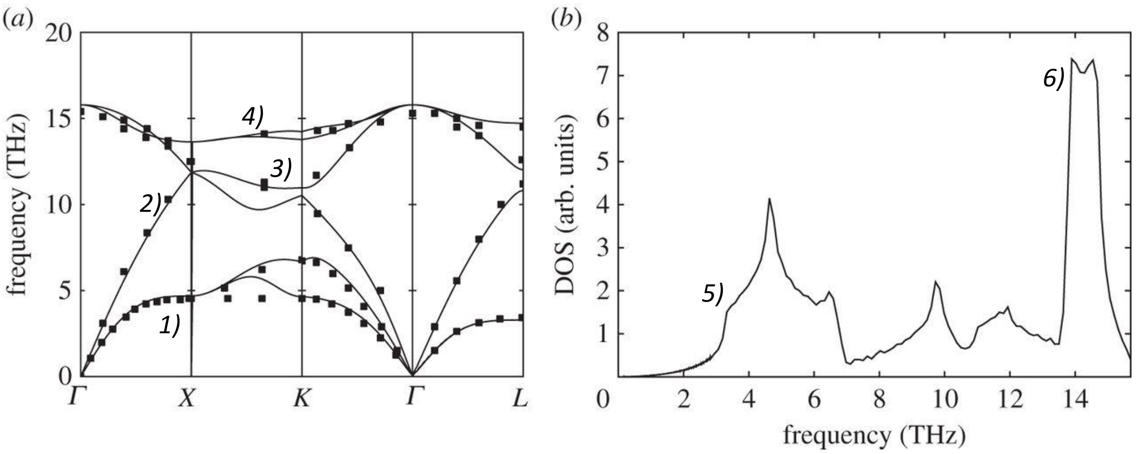
Problem 2

a) Sketch the dispersion relation for a 1-dimensional monoatomic chain of atoms. Why is there no optical branch?

Periodic boundary conditions lead to a restriction of the possible *k*-values. Assume a linear chain of copper atoms (atomic mass 63.5 u), of length 1.0 mm. The lattice spacing is 3.6 Å and the force constant 50 N m^{-1}.

b) What is the smallest possible wave number *k*?
What is the corresponding energy in electron volts?
(Assume periodic boundary conditions).

The phonon dispersion relation and corresponding density of states for silicon is given in the figure below (the squares indicate experimental measurement points):



c) Explain the features marked 1) – 4) in the dispersion relation. As usual, *Γ* denotes the origin of the Brillouin zone, and *X* and *K* are high-symmetry points on the 1st Brillouin zone boundary.
Can silicon crystals have optical phonons?

d) Derive the density of states $D(\omega)$ in the Debye approximation in 3D. Comment on the features marked 5) and 6) in the plot of the density of states.

Problem 3

a) Si is known to be a semiconductor with an indirect bandgap of 1.1 eV.
Explain how electrons can be excited across the bandgap for energies near the value 1.1 eV, and sketch the light absorption curve as function of photon energy that would be measured with a spectrophotometer. At what photon wavelength is the indirect bandgap?

b) The electron density *n* in the conduction band is given by

$$n = \frac{1}{\sqrt{2}}\left(\frac{m_e^* k_B T}{\pi\hbar^2}\right)^{3/2} e^{-(E_g-\mu)/k_BT} \; .$$

Explain the main steps in the derivation of this expression. Then write down the corresponding expression for the hole density *p* in the valence band, and show that

$$np = 4A \;\; m_e^* m_h^* {}^{\;3/2} \; e^{-E_g/k_BT} \; .$$

Find an expression for the constant *A*.

c) What is meant by an *intrinsic* semiconductor? If we for simplicity assume $m_e^* = m_h^* = m_e$, what are the intrinsic carrier concentrations n_i and p_i at T = 150 K and at T = 300 K?

d) Show that if we assume $n = p$, the chemical potential is given by

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

Comment on the answer. *Hint*: k_BT ~ 0.025 eV at room temperature.
Does Si have a Fermi surface?

Attachment

Some expressions and constants that may prove useful:

Physical constants

One mole: $M(^{12}C) = 12$ g	$1u = 1.6605 \cdot 10^{-27}$ kg	$N_A = 6.0221 \cdot 10^{23}$ mol^{-1}
$k_B = 1.3807 \cdot 10^{-23}$ J/K	$R = N_A\, k_B = 8.3145$ J mol^{-1} K^{-1}	0°C = 273.15 K
$\varepsilon_0 = 8.8542 \cdot 10^{-12}$ C^2/Nm^2	$\mu_0 = 4\pi \cdot 10^{-7}$ N/A^2	
$e = 1.6022 \cdot 10^{-19}$ C	$m_e = 9.1094 \cdot 10^{-31}$ kg	
$c = 2.998 \cdot 10^8$ m/s	$h = 6.6261 \cdot 10^{-34}$ Js	$g = 9.81$ m/s^2

Mean occupation number for fermions

$$f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1}$$

Mean occupation number for bosons

$$f(\omega) = \frac{1}{e^{\hbar\omega/k_B T} - 1}$$

Density of states for free electrons ($E(k) = E_0 + \hbar^2 k^2 / 2m$):

$$D(E) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} (E - E_0)^{\frac{1}{2}}$$

Phonon dispersion relation for a monoatomic basis:

$$\omega^2 = \frac{4\alpha}{M}\sin^2\frac{ka}{2}$$