

## **Midterm Examination in FYS3410**

30.03.2009

Duration: 3 hours

No in-advance prepared helping materials are allowed to be used during the examination. No books are allowed except standard reference books listing mathematical formulas if needed. Calculators are allowed.

The present examination measures the level of understanding reached by students on 4 core introductory topics of Solid State Physics as addressed in the lectures/seminars within FYS3410 and in accordance with the course syllabus based on selective chapters of Kittel's book. All examination questions are organized within the following topics:

1. Crystalline lattice and x-ray diffraction
2. Point defects and stress
3. Vibrations and phonons
4. Free electron Fermi gas

Each topic contains question of different levels of complexity and a full answer to each topic provides 25% of a full score.

## FYS3410 Topic 1: Crystalline lattice and x-ray diffraction

1.1 How Miller indices are defined?

1.2 Consider planes A, B, C, D, E, F of the lattice shown in Fig.1. The Miller indices for plane A are (001). What are Miller indices for planes B, C, D, E, F?

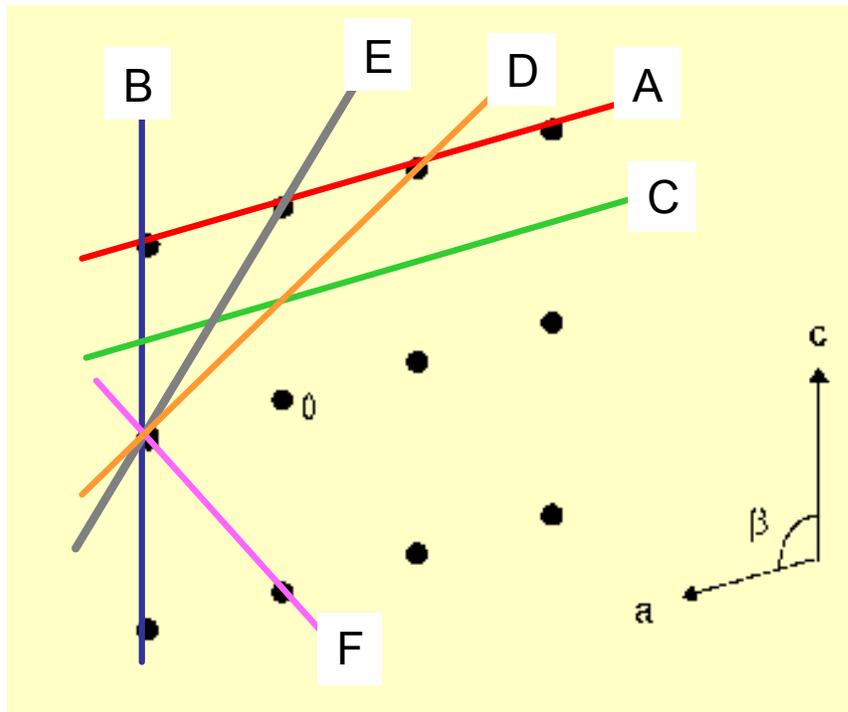


Fig.1. Three-dimensional lattice with basis vectors  $\vec{a}$ ,  $\vec{b}$ ,  $\vec{c}$  and the origo is marked with "0". Vectors  $\vec{a}$  and  $\vec{c}$  are directed as shown at the right hand side of the figure. Vector  $\vec{b}$  is normal to the page plane and is directed toward the reader.

1.3 Show that the diffraction pattern obtained from a crystal corresponds to reciprocal lattice points and maps hkl-families of planes in real space. Tips: (i) use the fact that the reciprocal

lattice vector  $\vec{G} = \frac{2\pi}{d_{hkl}} \vec{n}_{hkl}$ , where  $\vec{n}_{hkl}$  is a normal to a hkl-plane and  $d_{hkl}$  is a distance

between hkl-planes; (ii) consider Bragg diffraction of a wave at a hkl-plane in terms of wave vector change ( $\Delta\vec{k}$ ) and develop Laue condition for diffraction; (iii) use Ewald construction for clarifications.

## FYS3410 Topic 2: Point defects and stress

2.1. Fig.2 illustrates the fact that it is energetically favourable having vacancies in a crystal at a concentration of  $n_{eq}$ . Explain (shortly, probably in one sentence) why the enthalpy/entropy increases/decreases with increasing number of vacancies in the crystal.

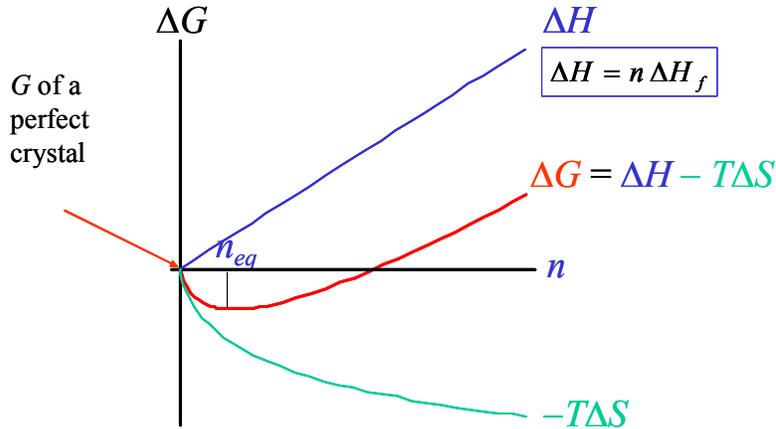


Fig.2. Illustration of the Gibbs free energy change ( $\Delta G$ ) with increasing number of vacancies ( $n$ ) in a crystal.

2.2 An introduction of  $n$  vacancies in a crystal having  $N$  atomic sites results in an increase of the number of indistinguishable states ( $W$ ) for the system and it can be readily shown that

$$W = \frac{N!}{(N-n)!n!}. \text{ The increase of } W \text{ results in an increase in the entropy of the system}$$

$S = k_B \ln W$ , known as a configurational entropy of the system. Derive the expression for

equilibrium vacancy concentration  $n_{eq}$  accounting for the enthalpy and configurational entropy changes when introducing vacancies into the crystal. Stirling's formula

$\ln X! \approx X \ln X - X$  is valid for large  $X$  and is to be applied simplifying the entropy calculation. We also assume that the amount of vacancies is much smaller than the amount of matrix atoms so that  $n \ll N$  holds.

2.3. The enthalpy of a vacancy formation is given by  $\Delta H_f = \Delta E_f + \sigma \Delta V_f$  where  $\Delta E_f$  and  $\Delta V_f$  are the formation energy and volume for a vacancy, respectively, while  $\sigma$  is the stress/pressure applied on the crystal. Assuming  $\Delta E_f = 2 \text{ eV}$  and  $\Delta V_f = 20 \text{ \AA}^3$  calculate vacancy concentration in such crystal at 300 and 800K at atmospheric pressure (assume atomic density of  $5 \times 10^{22} \text{ cm}^{-3}$ ).

2.4. Continue study the same crystal as in 2.3. What pressure/stress has to be applied on the crystal (assume purely hydrostatic case) at 300K resulting in vacancy concentration as it is established at 800K at atmospheric pressure? What pressure/stress was applied – tensile or compressive?

Note,

$$1 \text{ \AA} = 10^{-8} \text{ cm}$$

$$1 \text{ atm} = 101.325 \text{ kPa}$$

$$1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$$

$$\text{Boltzmann constant } k_B = 8.617 \times 10^{-5} \text{ eV/K}$$

### FYS3410 Topic 3: Vibrations and phonons

3.1 Assuming one atom (of mass  $m$ ) per primitive cell available in a crystal. The dispersion law is given by  $\omega^2 = \frac{4c}{m} \sin^2 \frac{ka}{2}$ . Analyze and sketch the dispersion law in the first Brillouin zone (BZ).

3.2 Analyse and sketch the group velocity corresponding to the vibrations described in 3.1. Importantly, show that the group velocity is zero at the boundary of the BZ. Explain the physics behind this.

3.3 Show that the density of states for phonons,  $D(\omega)$ , in one dimension is given by

$D_1(\omega) = \frac{L}{\pi} \frac{dk}{d\omega}$ . Take into account that the quantization of  $k$  follows from boundary

conditions. Tips: calculate the number of modes per unit  $k$

3.4 Explain the specific features of the Einstein and Debye models for lattice heat capacitance. What are the physical assumptions behind these models?

#### FYS3410 Topic 4: Free Electron Fermi gas (FEFG)

4.1 The free electron Fermi gas is described in terms of an independent electron orbital model, where the orbitals (electron states) are to a large extent determined by boundary conditions. The electrons are modelled as living in a box having a sidelength  $L$  and the potential inside the box is zero. Show that the allowed energy states (orbitals) in one dimension are expressed

$$\text{by } \varepsilon_n = \frac{\hbar^2}{2m} \left( \frac{\pi \cdot n}{L} \right)^2.$$

4.2 The Fermi energy is defined as the topmost filled level in the ground state of an  $N$  electron free Fermi gas. What is the Fermi energy ( $\varepsilon_F$ ) in one dimension? Remember the Pauli principle!

4.3 In three dimensions  $\varepsilon_F = \frac{\hbar^2}{2m} \left( \frac{3\pi^2 \cdot N}{V} \right)^{2/3}$ . Derive and sketch the density of states,  $D(\varepsilon)$ ,

for three dimensional FEFG in the ground state. Accounting for the Fermi-Dirac distribution

$$f(\varepsilon, \mu, T) = \frac{1}{\exp\left(\frac{\varepsilon - \mu}{k_B T}\right) + 1}$$

density of states changes with increasing temperature.

4.4 Using your plot obtained in 4.3, explain qualitatively the fact that the heat capacity of the FEFG is much lower than that of an ideal monoatomic gas. Tips: account for the fact that in FEFG only electrons within a range  $k_B T$  around  $\varepsilon_F$  are excited at a temperature  $T$ .