STOCKHOLMS UNIVERSITET
FYSIKUM

Solutions

Examination in Condensed Matter Physics I, FK3004, 7.5 hp
Friday, June 11, 2010, 09.00-15.00.

Allowed help:
- periodic table and fundamental constants (distributed)
- formula sheet (distributed)
- pocket calculator, BETA / mathematics handbook or similar

Instructions:
All solutions should be easy to read and have enough details to be followed. The use of nontrivial formulas from the formula sheet should be explained. *Summarize each problem* before its solution, so that the solution becomes self-explained. State any assumptions or interpretation of a problem formulation.

Good luck! / A.R.

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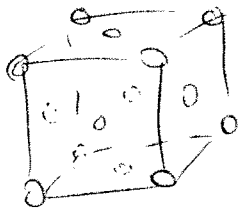
1. **a)** A certain metal has a monoatomic *fcc* structure with a lattice parameter $a_{\text{fcc}} = 3.638\,\text{Å}$ at $T = 1080\,\text{K}$. At the higher temperature $T = 1680\,\text{K}$, the structure has changed to *bcc*, with a lattice parameter $a_{\text{bcc}} = 2.936\,\text{Å}$. How much does the density change when going from 1080 K to 1680 K? (2p)
b) Define the reciprocal lattice and explain what the first Brillouin zone is. (2p)

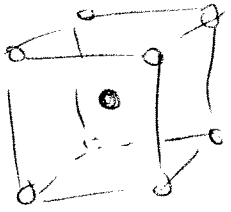
fcc has 4 at/cell:

$\frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$



bcc has 2 at/cell:

$\frac{1}{8} \times 8 + 1 = 2$



At 1080 K, the density is $\rho_{\text{fcc}} = \frac{4m}{a_{\text{fcc}}^3}$

At 1680 K — " — $\rho_{\text{bcc}} = \frac{2m}{a_{\text{bcc}}^3}$

$\Rightarrow \frac{\rho_{\text{bcc}} - \rho_{\text{fcc}}}{\rho_{\text{fcc}}} = \frac{1}{2}\left(\frac{a_{\text{fcc}}}{a_{\text{bcc}}}\right)^3 - 1 =$

$= -4.9\,\%$

1b) Reciprocal lattice:

Given a Bravais lattice $\bar{R} = n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3$ (n_i: integers; $\bar{a}_i$: primitive vectors of direct lattice)

the reciprocal lattice is
the set of all wave vectors $\bar{G}$
that fulfill

$$e^{i\bar{G}\cdot(\bar{r}+\bar{R})} = e^{i\bar{G}\cdot\bar{r}}$$

If we write $\bar{G} = h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3$ h,k,l integers

the above condition corresponds to $\bar{b}_i\cdot\bar{a}_j = 2\pi\delta_{ij}$

The $\bar{b}_i$'s can be obtained as $\bar{b}_1 = 2\pi\frac{\bar{a}_2\times\bar{a}_3}{\bar{a}_1\cdot(\bar{a}_2\times\bar{a}_3)}$ etc

First Brillouin zone:

The first B.Z. is the Wigner-Seitz cell of the reciprocal lattice.

A Wigner-Seitz cell is a primitive
unit cell that contains the space
closer to that cell center than to the center
of any neighboring cell.

2. A polycrystalline sample with bodycentered tetragonal structure was studied with monochromatic x-ray, $\lambda = 1.5405$ Å. The four lowest Bragg angles were measured to $\theta = 21.00°$, $22.06°$, $28.78°$, and $32.09°$.
a) Give an expression for a general reciprocal lattice vector $\mathbf{G}(hkl)$ for the tetragonal lattice, which has lattice vectors $a\hat{x}$, $a\hat{y}$, and $c\hat{z}$. (0.5p)
b) Start with the Laue condition $\Delta\mathbf{k} = \mathbf{G}$ and deduce the quadratic form for a tetragonal lattice. (1.5p)
c) For *bcc* structures, the allowed reflexes have $h+k+l = 2n$, where n is an integer. Motivate that this is also the case for the bodycentered tetragonal structure. (0.5p)
d) Determine the lattice parameters a and c. (1.5p)

See exam 2009-06-17, problem #3.

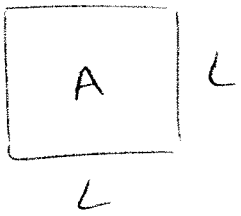
3. A two-dimensional free electron gas is contained in a square of area A. Show that the temperature dependence of the Fermi level (chemical potential) μ is given by

$$\mu(T) = k_B T \cdot \ln\left[\exp\left(\frac{n\pi\hbar^2}{mk_BT}\right) - 1\right]$$

where m is the electron mass and n is the number of electrons per area A. (4p)
Hint:

$$\int_0^\infty \frac{1}{\exp\left[(E-\mu)/k_BT\right]+1} dE = k_BT \cdot \ln\left[1+\exp\left(\mu/k_BT\right)\right]$$

Solution



Assume $A = L^2$

Periodic boundary cond.

$k_x = \frac{2\pi}{L} n_x \quad k_y = \frac{2\pi}{L} n_y \quad n_x, n_y$ integers

Density of k-points $= \frac{1}{\left(\frac{2\pi}{L}\right)^2} = \frac{A}{(2\pi)^2}$

Density of states (spin)

$$D(k)dk = \underbrace{2\pi k dk}_{\text{constant!}} \cdot \frac{A}{(2\pi)^2} \cdot 2 = \frac{A \cdot k}{\pi} dk = D(\varepsilon)d\varepsilon$$

$$\varepsilon = \frac{\hbar^2 k^2}{2m} \quad d\varepsilon = \frac{\hbar^2 k}{m} dk \quad \frac{A}{\pi}\frac{m}{\hbar^2} d\varepsilon = D(\varepsilon)d\varepsilon \quad D(\varepsilon) = \frac{m \cdot A}{\pi\hbar^2}$$

$$N = n \cdot A = \int_0^\infty f_{FD} \cdot D(\varepsilon)\, d\varepsilon = \frac{m \cdot A}{\pi\hbar^2} \int_0^\infty \frac{d\varepsilon}{e^{(\varepsilon-\mu)/k_BT}+1} = \frac{m \cdot A}{\pi\hbar^2} k_BT \cdot \ln\left[1+\ldots\right]$$

from hint

$$\Rightarrow \ln\left[1+\exp\left(\mu/k_BT\right)\right] = \frac{\pi\hbar^2 n}{mk_BT} \quad ; \quad 1+e^{\mu/k_BT} = e^{\pi\hbar^2 n/mk_BT}$$

$$\Rightarrow \mu = k_BT \cdot \ln\left[\exp\left(\frac{\pi\hbar^2 n}{mk_BT}\right) - 1\right]$$

4. Consider a one-dimensional crystal with 1 atom per primitive cell and a lattice parameter $a = 2\,\text{Å}$. The lattice vibrations in this crystal are harmonic with interaction only between nearest neighbors. In the long wavelength limit, i.e., for $K = 2\pi/\lambda \to 0$, the propagation velocity of the lattice waves is 115 m/s.

a) We know that lattice vibrations are quantized. In which interval of energy are the possible phonon energies found for an infinitely long crystal? Specify lower and upper boundaries in meV. (2p)

b) Now assume that the crystal is having a length $L = 100\,\text{nm}$. Estimate the lowest possible phonon energy (in meV). (2p)

Solution a) 1-dim crystal : $\omega = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{Ka}{2}\right)\right|$

$$v_s = \lim_{K\to 0}\frac{d\omega}{dK} = \frac{a}{2}\sqrt{\frac{4C}{m}} = 115\ \text{m/s}$$

Infinitely long crystal $\Rightarrow K_{min} = \frac{2\pi}{\lambda_{max}} = 0 \Rightarrow \omega_{min} = 0$

$\Rightarrow \varepsilon_{min} = 0$

$$K_{max} = \frac{\pi}{a} \Longleftrightarrow \omega = \omega_{max} = \sqrt{\frac{4C}{m}} = v_s\cdot\frac{2}{a}$$

$$\hbar\omega_{max} = \left\{\begin{matrix}\text{max}\\ \text{phonon}\\ \text{energy}\end{matrix}\right\} = \frac{2\hbar v_s}{a} = \frac{2\cdot 6.58\cdot 10^{-16}\ \text{eV·s}\cdot 115\ \text{m/s}}{2\cdot 10^{-10}\ \text{m}}$$

$$= 0.76\ \text{meV}$$

b) With $L = 100\,\text{nm} \Rightarrow \lambda_{max} \Longleftrightarrow \frac{1}{2}$ wavelength over L

$$\lambda_{max} = 2L$$

$$K_{min} = \frac{2\pi}{\lambda_{max}} = \frac{\pi}{L}$$

$$\omega_{min} \approx \sqrt{\frac{4C}{m}}\cdot\frac{Ka}{2} = v_s\cdot K_{min} = \frac{\pi v_s}{L}$$

$\sin x \approx x$ for small x

$$\hbar\omega_{min} = \frac{\pi\hbar v_s}{L} = \frac{\pi\cdot 6.58\cdot 10^{-16}\ \text{eV·s}\cdot 115\ \text{m/s}}{100\cdot 10^{-9}\ \text{m}}$$

$$= 2.37\cdot 10^{-3}\ \text{meV}$$

With periodic boundary conditions the result would differ by a factor 2

5. a) Discuss the experimental observation and interpretation of the de Haas – van Alphen effect. (2p)
b) Suppose that you are studying an unknown material. You are carrying out the following measurements:

A. Resistivity as a function of temperature.

B. Hall effect.

C. Optical absorption.

D. X-ray diffraction.

Explain how you would use the results of each of these measurements to improve your understanding of what kind of material you have. (2p)

Solution a) de Haas - van Alphen effect

Experiment: Measure oscillations in magnetization / susceptibility as a function of applied field

$\Rightarrow$ Oscillations with period in $\frac{1}{B}$

$$\underbrace{\Delta\left(\frac{1}{B}\right)}_{\text{period in } \frac{1}{B}} = \frac{e}{\hbar}\cdot\frac{1}{A_e}$$

A_e: extremal area of Fermi surface in plane normal to applied field

$\Rightarrow$ Fermi surface probe

b) Examples

$R(T)$: Metal, insulator, bandgap, superconductor?

Hall effect: Sign and number of charge carriers

Optical absorption: Band gap, defects

X-ray diffraction: Crystal structure, lattice parameters

6. a) Show how to obtain the Curie law, i.e., that the magnetic susceptibility $\chi \propto 1/T$, for a free spin paramagnet with $J = 1/2$. (2.5p)
b) Describe two types of crystal defects and their possible, practical importance. (1.5p)

Solution a) See exam 2007-03-30

b) Examples

		Practical importance
Vacancies:	Point defects with missing atoms	× Color of ionic crystals
Interstitials:	Extra atoms disturbing the lattice	× Electrical conductivity × Thermal conductivity
Dislocations:	Line defects	× Yield strength
Surface defects:	Twin boundaries Stacking faults Grain boundaries	× Pinning dislocations × Local anisotropy → global isotropic
Substitution impurities:	Point defects where one kind of atom is replaced by a different kind	Ex. × Zn atoms in brass