NTNU

Department of Physics

Examination paper for FY3114 Functional Materials and FY8912 Functional Materials

Academic contact during examination: Steinar Raaen

Phone: 482 96 758

Examination date: December 11, 2017

Examination time (from-to): 9:00-13:00

Permitted examination support material:

Alternative C, Approved pocket calculator

K. Rottmann: Mathematical formulas (or equivalent)

English dictionary

Language: English

Number of pages (front page excluded): 5

Number of pages enclosed: 0

Informasjon om trykking av eksamensoppgave

Originalen er:

1-sidig □ **2-sidig** □

sort/hvit □ **farger** □

skal ha flervalgskjema □

Checked by:

Date Signature

Students will find the examination results in Studentweb. Please contact the department if you have questions about your results. The Examinations Office will not be able to answer this.

Problem 1
Multiple choice questions.
Please select one out of the four alternatives.

1.1 A feature of topological insulators is
- **A.** that they are being used in quantum computers.
- **B.** high bulk conductance.
- **C.** high surface conductance.
- **D.** that they already have a range of applications.

1.2 Facts of graphene transistors are
- **A.** that fabrication methods are well developed.
- **B.** that the electron mobility may be almost as good as in silicon.
- **C.** candidates for even smaller electronic components.
- **D.** a band gap is not needed.

1.3 High-K dielectrics are characterized by
- **A.** low leakage currents.
- **B.** the possibility for scaling down to obtain high circuit density.
- **C.** that they cannot resist high electric fields.
- **D.** high electrical conductivity.

1.4 Features of the carbon nano-tube transistor include
- **A.** easy to fabricate.
- **B.** low thermal conductivity.
- **C.** low electrical conductivity.
- **D.** high electron mobility.

1.5 Which statement is correct regarding ferroelectric memory devices?
- **A.** they may be made from centrosymmetric materials.
- **B.** they have very high storage densities.
- **C.** they are well suited for low cost production.
- **D.** they may be used in non-volatile memory applications.

1.6 Organic semiconductor devices are characterized by:
- **A.** have high production costs.
- **B.** they possess a high degree of molecular orientation.
- **C.** they are promising for display technologies.
- **D.** the theoretical understanding is very good.

1.7 The spintronic transistor......
- **A.** may be fabricated at low cost.
- **B.** has already been commercialized.
- **C.** may be based on the spin Hall effect.
- **D.** uses less power but are slower than ordinary transistors.

1.8 Piezoelectric transistors.....
- **A.** are not suitable for use in touch devices.
- **B.** represent presently a mature technology.
- **C.** may be used as strain sensors.
- **D.** are likely to replace Si-based transistors in the future.

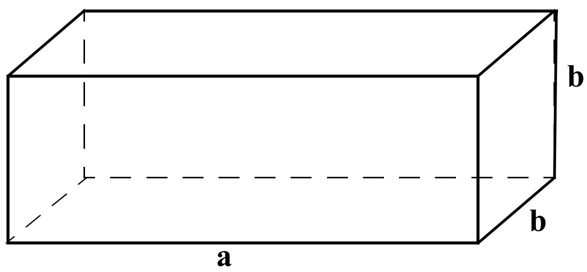
1.9 Graphene has the following property.....
- **A.** the natural band gap is about 1 eV.
- **B.** the effective mass is small.
- **C.** it is almost as strong as stainless steel.
- **D.** it is easy to fabricate for use in electronic devices.

1.10 Which one of the following statements is correct?
- **A.** a pyroelectric material is also ferroelectric
- **B.** a piezoelectric material is also ferroelectric
- **C.** the dielectric constant of a ferroelectric material is low
- **D.** a ferroelectric material is also pyroelectric and piezoelectric

Problem 2

2.1 How many 2D crystallographic point groups exist.
List the plane lattices that are possible.

2.2 In the figure below is shown a tetragonal box. List the symmetry elements of the box. How many symmetry elements are contained in the point group.



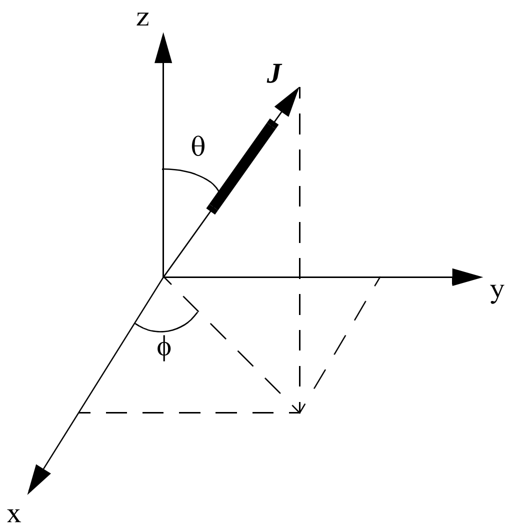
2.3 Draw the point group projections (stereogram) for the tetragonal box.

Problem 3
3.1
State Neumann's principle?
Show how a mirror in the yz-plane can be used to reduce the number of non-zero elements in a symmetric 2nd rank tensor.

3.2
Find the angle of rotation around the z-axis which diagonalize a symmetric 2nd rank tensor of a monoclinic system.

3.3

A hexagonal conducting material is shaped as a long thin rod, and is directed as shown in the figure below. The current ***J*** flows in the direction of the rod. The rod is at an angle $\theta = 30^\circ$ with the z-axis, and the projection of the rod into the xy-plane is at an angle $\phi = 45^\circ$ with the x-axis.



Find the electrical resistivity ρ_J along the direction of the current ***J*** in terms of the components of the resistivity tensor..

Problem 4

4.1 InP has band gap of 1.27 eV at a temperature of 300 K. Find the energy of the electron and hole (relative to the respective band edge) that results when a 1.5 eV photon is adsorbed.

4.2 A p-doped Si sample is at a temperature of 300 K. The density of holes in the valence band is p_a = $5 \cdot 10^{17}$ cm^{-3}. Use the law of mass action to find the conductivity due to the electrons. What is the conductivity due to the holes? Compare to the conductivity of an undoped sample.

4.3 The electrons in a Ga As material are moving in an electric field of 5 kV/cm. The carrier concentration is 10^{15} cm^{-3}. We assume that the drift velocity has saturated at 10^7 cm/s.
Calculate the drift current density. Estimate the scattering relaxation time τ_{sc}.
Calculate the concentration gradient for the case that the diffusion current has the same magnitude as the drift current. The diffusion coefficient is given to be 100 cm^2/s.

Problem 5

5.1 Give examples of applications where hard and soft ferromagnetic materials are used.

5.2 Give a brief description of the main characteristics of paramagnetic, antiferromagnetic, and ferromagnetic materials.

5.3 An electric field is applied in the *z*-direction of an electro-optic active cubic material of inversion symmetry. The index of refraction in the absence of an electric field is *n*. The influence of the electric field on the impermeability tensor is given by the Kerr effect:

$$\eta_{ij}(E) = \eta_{ij}^0 + \sum_{kl} s_{ijkl} E_k E_l \quad where \ \eta_{11}^0 = \eta_{22}^0 = \eta_{33}^0 = \frac{1}{n^2} \quad other \ \eta_{ij}^0 = 0$$

The only non-zero elements of the fourth rank tensor are $s_{11}=s_{22}=s_{33}$, $s_{12}=s_{13}=s_{23}$, $s_{44}=s_{55}=s_{66}$.
(using contracted notation). Write out the elements of the impermeability tensor.
Also find an expression for the index ellipsoid.

Some potentially useful constants and formulas

Constants and numerical values (densities and mobilities at 300 K):

$m_e = 9.1\cdot10^{-31}$ kg, $e = 1.6\cdot10^{-19}$ C, $k_B = 1.38\cdot10^{-23}$ J/K = $8.617\cdot10^{-5}$ eV/K, $h = 6.63\cdot10^{-34}$ Js

n_i(Si) = $1.5\cdot10^{10}$ cm^{-3}, μ_n(Si) = 1000 cm^2/Vs, μ_p(Si) = 350 cm^2/Vs (low field values)

n_i(GaAs) = $1.84\cdot10^{6}$cm^{-3}, μ_n(GaAs) = 8000 cm^2/Vs, μ_p(GaAs) = 400 cm^2/Vs (low field values)

m_e^*(GaAs) = 0.067m_e, m_h^*(GaAs) = 0.45m_e, m_e^*(Ge) = 0.56m_e, m_h^*(Ge) = 0.29m_e

m_e^*(Si) = 0.26m_e, m_h^*(Si) = 0.5m_e, m_e^*(InP) = 0.07m_e, m_h^*(InP) = 0.4m_e

Rotation matrix R:

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} \quad and \quad \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix}$$

Transformation of tensors:

$$T_{ij}' = \sum_{kl} R_{ik} R_{jl} T_{kl} \quad and \quad T_{ijk}' = \sum_{lmn} R_{il} R_{jm} R_{kn} T_{lmn}$$

Transformation of products of coordinates:

$$x_i' x_j' = \sum_{kl} R_{ik} R_{jl} x_k x_l \quad and \quad x_i' x_j' x_k' = \sum_{lmn} R_{il} R_{jm} R_{kn} x_l x_m x_n$$

Dielectric permittivity tensor:

$$\varepsilon_{triclinic} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33} \end{bmatrix} \quad \varepsilon_{monoclinic} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & 0 \\ \varepsilon_{12} & \varepsilon_{22} & 0 \\ 0 & 0 & \varepsilon_{33} \end{bmatrix} \quad \varepsilon_{orthorhombic} = \begin{bmatrix} \varepsilon_{11} & 0 & 0 \\ 0 & \varepsilon_{22} & 0 \\ 0 & 0 & \varepsilon_{33} \end{bmatrix}$$

$$\varepsilon_{tetragonal} = \varepsilon_{trigonal} = \varepsilon_{hexagonal} = \begin{bmatrix} \varepsilon_{11} & 0 & 0 \\ 0 & \varepsilon_{11} & 0 \\ 0 & 0 & \varepsilon_{33} \end{bmatrix} \quad \varepsilon_{cubic} = \begin{bmatrix} \varepsilon_{11} & 0 & 0 \\ 0 & \varepsilon_{11} & 0 \\ 0 & 0 & \varepsilon_{11} \end{bmatrix}$$

Conductivity, drift velocity, mobility, diffusion coefficient, and diffusion current for electron:

$$\sigma = ne^2\tau_{sc}/m^* = ne\mu \qquad \boldsymbol{v_d} = \mu\boldsymbol{E} \qquad \mu = e\tau_{sc}/m^* \qquad D_n = \mu_n k_B T/e \qquad J_{diff} = eD_n\frac{dn}{dx}$$

Electrons and holes in semiconductors:

$$n = N_c e^{-(E_c - E_F)/k_B T} \qquad p = N_v e^{-(E_F - E_v)/k_B T} \qquad np = N_c N_v e^{-E_{gap}/k_B T} \qquad N_c = 2\left(\frac{m_e^* k_B T}{h^2/2\pi}\right)^{3/2} \qquad N_v = 2\left(\frac{m_h^* k_B T}{h^2/2\pi}\right)^{3/2}$$

Emission:

$$\hbar\omega = E_e - E_h = E_{gap} + \frac{(\hbar k)^2}{2m_r^*} \qquad W_{em}^{st}(\hbar\omega) = \frac{e^2 n_r \hbar\omega}{3\pi\varepsilon_0 m_e^2 c^3 \hbar^2}|p_{cv}|^2 \cdot n_{ph}(\hbar\omega) \qquad \frac{2|p_{cv}|^2}{m_e} = 23eV \quad (GaAs)$$

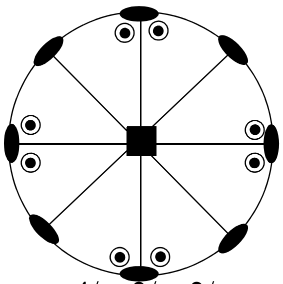
Solution Exam Dec.11, 2017.

Problem 1. Multiple choice questions: CCBDD CCCBD

Problem 2.
2.1. There are 10 2D crystallographic point groups. The 5 plane lattices are: oblique, rectangular, centered rectangular, square, hexagonal.

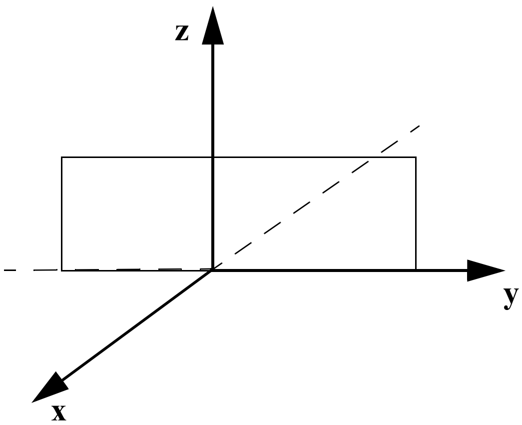
2.2. Symmetry elements for the tetragonal box: identity and inversion (1 and -1), four-fold rotation (4^1, 4^2, 4^3), 5 mirror planes, 4 two-fold rotation axes, four-fold rotation-inversion (-4^1 and -4^3, note that $-4^2 = 2$). A total of 16 symmetry elements.

2.3. Stereogram for the tetragonal box:



4/m 2/m 2/m

Problem 3
3.1
Neumann's principle states that a physical property of an anisotropic material must at least possess the symmetry of the crystallographic point group.
A mirror symmetry reduces the number of non-zero elements in a second rank tensor:



mirror in the yz-plane:
x' -> -x
y' -> y
z' -> z
Since a second rank tensor ε transforms as the product of two coordinates we get:
$\varepsilon'_{12} = -\varepsilon_{12}$
$\varepsilon'_{13} = -\varepsilon_{13}$
Since this is a symmetry operation we must have that $\varepsilon_{ij}' = \varepsilon_{ij}$
which means that $\varepsilon_{12} = \varepsilon_{13} = 0$.

3.2
Will diagonalize a 2nd rank monoclinic tensor by rotation.

$$\rho_{monoclinic} = \begin{bmatrix} \rho_{11} & \rho_{12} & 0 \\ \rho_{12} & \rho_{22} & 0 \\ 0 & 0 & \rho_{33} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

therefore $x'y' = (yy - xx)\sin\theta\cos\theta + xy(\cos\theta\cos\theta - \sin\theta\sin\theta)$

and $\rho'_{12} = (\rho_{22} - \rho_{11})\dfrac{\sin 2\theta}{2} + \rho_{12}\cos 2\theta$

For $\rho'_{12} = 0$ we get:

$$\tan 2\theta = \frac{2\rho_{12}}{\rho_{11} - \rho_{22}}$$

3.3

The resistivity tensor of a hexagonal solid is given by

$$\rho_{monoclinic} = \begin{bmatrix} \rho_{11} & 0 & 0 \\ 0 & \rho_{11} & 0 \\ 0 & 0 & \rho_{33} \end{bmatrix} \quad and \quad \begin{bmatrix} E_1 \\ E_2 \\ E_3 \end{bmatrix} = \begin{bmatrix} \rho_{11} & 0 & 0 \\ 0 & \rho_{11} & 0 \\ 0 & 0 & \rho_{33} \end{bmatrix} \begin{bmatrix} J_1 \\ J_2 \\ J_3 \end{bmatrix}$$

The resistivity along the direction of the electric current is given by

$$\rho_J = E_J / J = \frac{\boldsymbol{E} \cdot \boldsymbol{J}}{J^2} = \sum_i E_i J_i / J^2 = \sum_{ij} \rho_{ij} \frac{J_j}{J} \frac{J_i}{J}$$

then we get

$$\rho_J = \rho_{11}\left(\frac{J_x}{J}\right)^2 + \rho_{11}\left(\frac{J_y}{J}\right)^2 + \rho_{33}\left(\frac{J_z}{J}\right)^2$$

From the figure we see

$$J_x = J \sin\theta \cos\phi \qquad J_y = J \sin\theta \sin\phi \qquad J_z = J \cos\theta$$

which gives when $\theta = 30^o$ and $\phi = 45^o$

$$\rho_J = \rho_{11}(\sin\theta\cos\phi)^2 + \rho_{11}(\sin\theta\sin\phi)^2 + \rho_{33}(\cos\theta)^2$$

$$\rho_J = \rho_{11}\left(\frac{1}{2}\frac{1}{\sqrt{2}}\right)^2 + \rho_{11}\left(\frac{1}{2}\frac{1}{\sqrt{2}}\right)^2 + \rho_{33}\left(\frac{\sqrt{3}}{2}\right)^2 = \frac{\rho_{11}}{4} + \frac{3\rho_{33}}{4}$$

Problem 4

4.1

A photon is absorbed by InP and thus creates an electron in the conduction band and a hole in the valence band. By using the reduced mass we may write

$$\hbar\omega = E_e - E_h = E_{gap} + \frac{(\hbar k)^2}{2m_r^*} \quad and \quad E_e = E_c + \frac{(\hbar k)^2}{2m_e^*} \quad and \quad E_h = E_v - \frac{(\hbar k)^2}{2m_h^*}$$

The energies of the electron and hole become

$$E_e - E_c = \frac{m_r^*}{m_e^*}(\hbar\omega - E_{gap}) = \frac{0,06}{0,07}(1,5 - 1,27) = 0,20eV$$

$$E_h - E_v = -\frac{m_r^*}{m_h^*}(\hbar\omega - E_{gap}) = \frac{-0,06}{0,4}(1,5 - 1,27) = -0,034eV$$

4.2

The conductivity is given by

$$\sigma = \sigma_n + \sigma_p = ne\mu_n + pe\mu_p = p_a e\mu_p + \frac{n_i^2}{p_a}e\mu_n = 28\frac{1}{\Omega cm} + 7,2 \cdot 10^{-14}\frac{1}{\Omega cm}$$

where the law of mass action has been used:

$$n \cdot p = n_i^2$$

The conductivities are

$$\sigma_n = 7,2 \cdot 10^{-14} \qquad \sigma_p = 28,0 \qquad \sigma_{intrinsic} = n_i e\mu_n + p_i e\mu_p = 3,2 \cdot 10^{-6}\frac{1}{\Omega cm}$$

4.3

Drift current, diffusion current and scattering relaxation time is given by:

$$J_{drift} = nev_{drift} = 1600\frac{cm}{s} \quad and \quad J_{diff} = eD_n\frac{dn}{dx} \qquad \tau_{sc} = \frac{m^* v_{drift}}{eE}$$

$$J_{drift} = J_{diff} \quad \Rightarrow \quad \frac{dn}{dx} = \frac{nv_{drift}}{D_n} = 1 \cdot 10^{20}\ cm^{-4} \qquad \tau_{sc} = 7,6 \cdot 10^{-10} s$$

Problem 5

5.1
Uses of hard ferromagnetic materials: permanent magnets, motors, induction ovens, magnetic recording.
Uses of soft ferromagnetic materials: transformers, flux guides, magnetic shielding

5.2
Paramagnetic: spins are randomly oriented in the absence of a magnetic field, no magnetic moment in the absence of a magnetic field, magnetic susceptibility is small and positive
Antiferromagnetic: spins are aligned antiparallel in the absence of a magnetic field, no magnetic moment in the absence of a magnetic field, magnetic susceptibility is small and positive
Ferromagnetic: spins are aligned in the absence of a magnetic field, magnetic moment in the absence of a magnetic field, magnetic susceptibility diverges at the critical temperature

5.3
The elements of the impermeability tensor may be written:

$$\eta_{11} = \eta_1 = \frac{1}{n^2} + s_{1133}E^2 = \frac{1}{n^2} + s_{13}E^2 = \frac{1}{n^2} + s_{12}E^2$$

$$\eta_{22} = \eta_2 = \frac{1}{n^2} + s_{2233}E^2 = \frac{1}{n^2} + s_{23}E^2 = \frac{1}{n^2} + s_{12}E^2$$

$$\eta_{33} = \eta_3 = \frac{1}{n^2} + s_{3333}E^2 = \frac{1}{n^2} + s_{33}E^2 = \frac{1}{n^2} + s_{11}E^2$$

The index ellipsoide may thus be written ($s_{13}=s_{23}=s_{12}$ and $s_{33}=s_{11}$):

$$\eta_{11}x^2 + \eta_{22}y^2 + \eta_{33}z^2 = 1$$

$$\left(\frac{1}{n^2} + s_{12}E^2\right)x^2 + \left(\frac{1}{n^2} + s_{12}E^2\right)y^2 + \left(\frac{1}{n^2} + s_{11}E^2\right)z^2 = 1$$

Or rewriting:

$$\frac{1}{n^2} + s_{12}E^2 = \left(\frac{n^2}{1 + s_{12}n^2E^2}\right)^{-1} = \left(\frac{n}{\sqrt{1 + s_{12}n^2E^2}}\right)^{-2} = \left[n\left(1 - \tfrac{1}{2}s_{12}n^2E^2\right)\right]^{-2} = \frac{1}{n_o^2}$$

$$\frac{1}{n^2} + s_{11}E^2 = \frac{1}{n_e^2}$$

$$\frac{x^2}{n_o} + \frac{y^2}{n_o} + \frac{z^2}{n_e} = 1$$

where n_o and n_e are the ordinary and extraordinary indices of refraction.