NTNU – Trondheim
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Department of physics

Examination paper for FY3114 Functional Materials

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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: 6

Checked by:

Date Signature

Problem 1

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

1.1 What is an advantage by using ferroelectric memory devices?
A. Low energy consumption for writing operations.
B. Low leakage currents.
C. Reading is a non-destructive operation.
D. Centrosymmetric materials may be used.

1.2 Which property characterizes graphene?
A. It is almost as strong as stainless steel.
B. The natural bandgap is about 1 eV.
C. Zero effective mass.
D. Easy to fabricate for use in electronic devices.

1.3 A property of high-κ dielectrics used in transistors is:
A. Reduced charge density at opposite sides of the dielectric.
B. Degraded channel carrier mobility.
C. Reduced phonon scattering.
D. Increased leakage current.

1.4 Organic semiconductor devices are characterized by:
A. High molecular orientation.
B. High production costs.
C. Easy to process.
D. Good theoretical understanding.

1.5 Strain effects on transistors result in:
A. Lifting of degenerate energy levels.
B. Reduce the mobility of electrons and holes.
C. Increased phonon scattering.
D. Surface roughness does not contribute to electron scattering.

1.6 Piezoelectric transistors:
A. may be made from centrosymmetric materials.
B. may be based on ZnO nanowires.
C. the gate voltage must be controlled by an electrical signal.
D. represent presently a mature technology.

1.7 Multiferoic devices:
A. may be made from metallic, semiconducting or insulating materials.
B. may be made from perovskites
C. are not suitable for storage devices.
D. suitable ordering temperatures for storage devices are well below room tempeatrure.

1.8 The following property is determined directly by the electrons and their interactions:
- **A.** ferroelectricity
- **B.** ferromagnetism
- **C.** piezoelectricity
- **D.** elastic properties

1.9 Which of the following crystal systems is uniaxial?:
- **A.** cubic
- **B.** tetragonal
- **C.** orthorombic
- **D.** moniclinic

1.10 Which one of these elemental materials is not ferromagnetic?:
- **A.** Fe
- **B.** Co
- **C.** Mn
- **D.** Ni

Problem 2

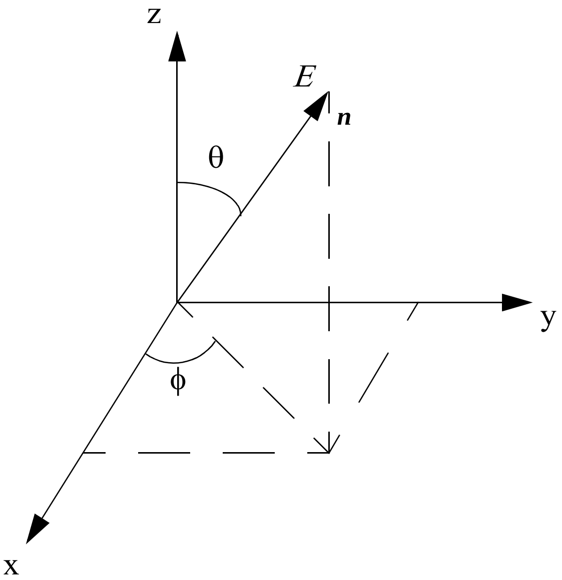
2.1 Please state Neumann's principle.
Which are the 5 crystallographic point symmetry operations?

2.2 Draw point group projections (stereograms) for the orthorombic point groups 222 and 2/m2/m2/m and the hexagonal group 32.

2.3 How many symmetry elements is contained in the point group of the regular tetrahedron? Please list these symmetry elements.

Problem 3

3.1



A trigonal material is cut into a slab where the normal is at an angle θ = 30° with the z-axis. The projection of the slab normal into the xy-plane is at an angle ϕ = 45° with the x-axis. The electric field ***E*** is in the direction of the slab normal (see the figure above). Find the dielectric permittivity ε_E along the direction of the electric field ***E***.

3.2

The resistivity tensor ρ of a monoclinic crystal is given by:

$$\rho = \begin{bmatrix} 3{,}9 & 6{,}5 & 0 \\ 6{,}5 & 1{,}3 & 0 \\ 0 & 0 & 5{,}2 \end{bmatrix} \qquad \textit{and} \qquad \mathbf{E} = \rho \mathbf{J}$$

in units of 10^{-8} Ωm.

This tensor can be diagonalized by rotation by an angle θ around the z-axis. Find the angle θ.

Problem 4

4.1 The effective mass of the electrons in a Si semiconductor is $m^* = 0.26m_e$. The optical phonon energy is $5\cdot10^{-2}$ eV. The electron scattering rate is $r_{sc} = 1/\tau_{sc} = 1\cdot10^{13}\ \mathrm{s}^{-1}$ at a temperature of 300 K. The average electron energy may be written as:

$$\varepsilon = \frac{3}{2}k_BT + \frac{1}{2}m^*v_d^2$$

Calculate the electric field at which phonons start to emit at temperature 300 K.

4.2 Consider a doped Si crystal where $N_D = 2\cdot10^{17}\ \mathrm{cm}^{-3}$. Assume that half of the donor atoms are ionized at a temperature of 300 K. Calculate the conductivity of the sample and compare to an undoped sample of Si. What is the conductivity due to the holes?

4.3 The electric field in a GaAs device of dimension 2μm is 5 kV/cm. Calculate the transit time for an electron through the device by using the low field value as well as the saturation drift velocity of $1\cdot10^{7}$ cm/s. Please comment on the results.

Problem 5

5.1 Consider a metal-semiconductor junction where the workfunction of the metal is larger than the workfunction of the semiconductor. Assume an n-doped semiconductor and sketch the energy level diagrams and discuss the charge carrier concentration at the junction. What is this junction called? What is the barrier height?

5.2 A 2eV photon is absorbed by a valence band electron in GaAs where the band gap is 1.4eV. Calculate the energy of the electron and hole that results from the absorption process.

5.3 α-Quartz is represented by the trigonal point group 32. The Piezoelectric tensor is given by:

$$d = \begin{bmatrix} 2{,}3 & -2{,}3 & 0 & 0{,}67 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0{,}67 & -4{,}6 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

in units of 10^{-12} C/N. Calculate the polarization along x, y and z axes for:

(a) Normal stress $\sigma = 2\cdot10^{4}\ \mathrm{N/m^2}$ along the x-axis.

(b) Shear stress $\sigma = 2\cdot10^{4}\ \mathrm{N/m^2}$ around the x-axis.

Some potentially useful constants and formulas

Constants:

$m_e = 9.1 \cdot 10^{-31}$ kg, $e = 1.6 \cdot 10^{-19}$ C, $k_B = 1.38 \cdot 10^{-23}$ J/K $= 8.617 \cdot 10^{-5}$ eV/K, $h = 6.63 \cdot 10^{-34}$ Js

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

n_i(GaAs) $= 1.84 \cdot 10^{6}$cm^{-3}, μ_n(GaAs) $= 8000$ cm^2/Vs, μ_p(GaAs) $= 400$ cm^2/Vs (low field values)

m_e^*(GaAs) $= 0.067 m_e$, m_h^*(GaAs) $= 0.45 m_e$

Rotation matrix *R*:

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

Transformation of tensors:

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

Transformation of products of coordinates:

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

Magnitude of ***D*** along ***E***:

$$D_E = \frac{\boldsymbol{D} \cdot \boldsymbol{E}}{E} = \sum_i D_i E_i / E = \sum_{ij} \varepsilon_{ij} E_j E_i / E \qquad and \qquad \varepsilon_E = D_E / E$$

Dielectric permittivity tensor:

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

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

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

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

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:

$$\hbar\omega = E_e - E_h = E_{gap} + \frac{(\hbar k)^2}{2 m_r^*} \qquad W_{em}^{st}(\hbar\omega) = \frac{e^2 n_r \hbar\omega}{3\pi\varepsilon_0 m_0^2 c^3 \hbar^2} |p_{cv}|^2 \cdot n_{ph}(\hbar\omega) \qquad \frac{2|p_{cv}|^2}{m_0} = 23eV \quad (GaAs)$$

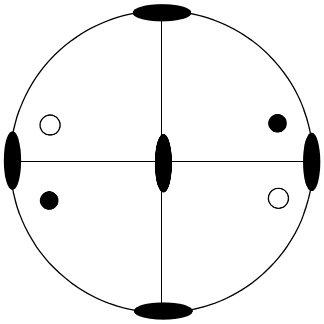
Solution Exam Dec.11, 2014

Problem 1. Multiple choice qusetions: ACBCA BBBBC

Problem 2.

2.1. Neumann's principle: *The symmetry elements of any physical property of a crystal must include the symmetry elements of the point group of the crystal.*

2.2. Stereograms



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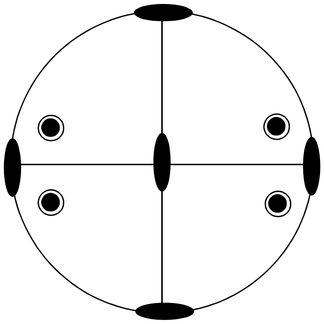
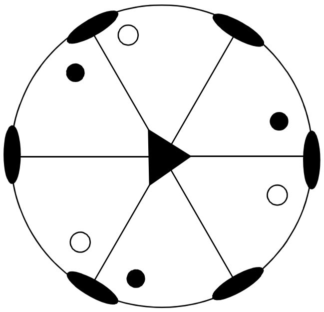
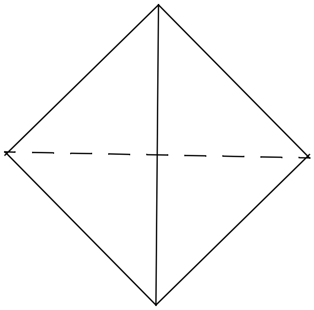


2/m 2/m 2/m



32

2.3. Regular tetrahedron



1 - identity

m - mirror plane (6 planes)

2 - 2-fold rotation (3 axes)

3 - 3-fold rotation (4 axes)

$\bar{4}$ - 4-fold rotation-inversion (3 axes)

$\bar{4}^3$ - twice 4-fold rotation-inversion (3 axes)

A total of 24 symmetry elements.

Problem 3

3.1

The dielectric tensor of a trigonal solid is given by

$$\varepsilon_{trigonal} = \begin{bmatrix} \varepsilon_{11} & 0 & 0 \\ 0 & \varepsilon_{11} & 0 \\ 0 & 0 & \varepsilon_{33} \end{bmatrix}$$

The dielectric permittivity alonf the electric field is given by

$$\varepsilon_E = D_E/E = \frac{\boldsymbol{D}\cdot\boldsymbol{E}}{E^2} = \sum_i D_i E_i/E^2 = \sum_{ij} \varepsilon_{ij} E_j E_i/E^2$$

then we get

$$\varepsilon_E = \varepsilon_{11}\left(\frac{E_x}{E}\right)^2 + \varepsilon_{11}\left(\frac{E_y}{E}\right)^2 + \varepsilon_{33}\left(\frac{E_z}{E}\right)^2$$

From the figure we see

$$E_x = E\sin\theta\cos\phi \qquad E_y = E\sin\theta\sin\phi \qquad E_z = E\cos\theta$$

which gives

$$\varepsilon_E = \varepsilon_{11}(\sin\theta\cos\phi)^2 + \varepsilon_{11}(\sin\theta\sin\phi)^2 + \varepsilon_{33}(\cos\theta)^2 = \varepsilon_{11}\sin\theta^2 + \varepsilon_{33}\cos\theta^2 = \varepsilon_{11}\left(\frac{1}{2}\right)^2 + \varepsilon_{33}\left(\frac{\sqrt{3}}{2}\right)^2 = \frac{1}{4}(\varepsilon_{11} + 3\varepsilon_{33})$$

3.2

Given the resistivity tensor ρ and the rotation matric R

$$\rho = \begin{bmatrix} 3{,}9 & 6{,}5 & 0 \\ 6{,}5 & 1{,}3 & 0 \\ 0 & 0 & 5{,}2 \end{bmatrix} \qquad a = \begin{bmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

we may write for the transformed tensor ρ’ after a rotation by an angle θ

$$\rho'_{ij} = \sum_{kl} a_{ik} a_{jl} \rho_{kl}$$

for the tensor to be diagonal we require elements 1,2 and 2,1 to be zero (symmetric tensor), and we may write

$$\rho'_{12} = a_{11}a_{21}\rho_{11} + a_{12}a_{21}\rho_{21} + a_{13}a_{21}\rho_{31} + a_{11}a_{22}\rho_{12} + a_{12}a_{22}\rho_{22} + a_{13}a_{32}\rho_{32} + a_{11}a_{23}\rho_{13} + a_{12}a_{23}\rho_{23} + a_{13}a_{33}\rho_{33}$$

inserting valves for the elements in the rotation matrix

$$\rho'_{12} = \cos\theta(-\sin\theta)\rho_{11} + \sin\theta(-\sin\theta)\rho_{21} + \cos\theta\cos\theta\rho_{12} + \sin\theta\cos\theta\rho_{22} = 0$$

which gives

$$\sin\theta\cos\theta(\rho_{22} - \rho_{11}) + \rho_{12}(\cos\theta^2 - \sin\theta^2) = \frac{1}{2}\sin 2\theta(\rho_{22} - \rho_{11}) + \rho_{12}\cos 2\theta = 0$$

and

$$\tan 2\theta = \frac{2\rho_{12}}{\rho_{11} - \rho_{22}} = 5 \qquad and \qquad \theta = 39{,}4^0$$

Problem 4

4.1

The drift velocity may be found by

$$\varepsilon = \frac{3}{2}k_BT + \frac{1}{2}m^*v_d^2 \Rightarrow \frac{1}{2}m^*v_d^2 = \varepsilon - \frac{3}{2}k_BT = 50meV - 39meV = 11meV \Rightarrow v_d = 1{,}22\cdot 10^5\frac{m}{s}$$

the electric field is then given by

$$\boldsymbol{v_d} = \mu\boldsymbol{E} = e\tau_{sc}E/m^* \Rightarrow E = \frac{\boldsymbol{v_d}m^*}{e\tau_{sc}} = r_{sc}\boldsymbol{v_d}m^*/e = 1{,}8\cdot 10^6 V/m$$

4.2

The conductivity is given by

$$\sigma = \sigma_n + \sigma_p = ne\mu_n + pe\mu_p = \frac{1}{2}N_De\mu_n + \frac{n_i^2}{\frac{1}{2}N_D}e\mu_p = 16\frac{1}{\Omega cm} + 1{,}3\cdot 10^{-13}\frac{1}{\Omega cm} = 16\frac{1}{\Omega cm}$$

and the hole conductivity is

$$\sigma_p = 1{,}3\cdot 10^{-13}\frac{1}{\Omega cm}$$

4.3

The transit time through the device is given by

$$t = \frac{L}{v_d} \qquad and \qquad \boldsymbol{v_d}(lowfield) = \mu_nE = 8000\cdot 5000\frac{cm}{s} = 4\cdot 10^7\frac{cm}{s} \qquad and \qquad \boldsymbol{v_d}(highfield) = 1\cdot 10^7\frac{cm}{s}$$

therefore

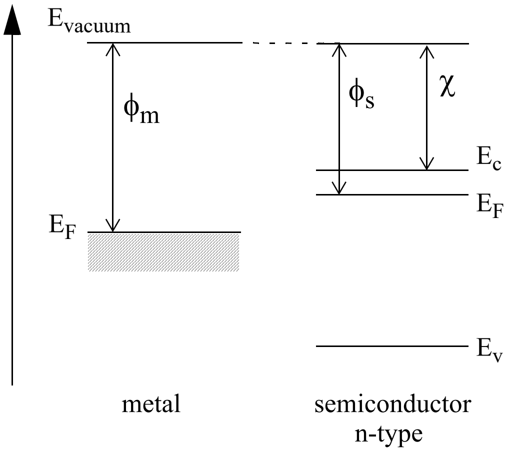
$$t(lowfield) = \frac{2\cdot 10^{-4}}{4\cdot 10^7}s = 5\cdot 10^{-12}s \qquad and \qquad t(highfield) = \frac{2\cdot 10^{-4}}{1\cdot 10^7}s = 20\cdot 10^{-12}s$$

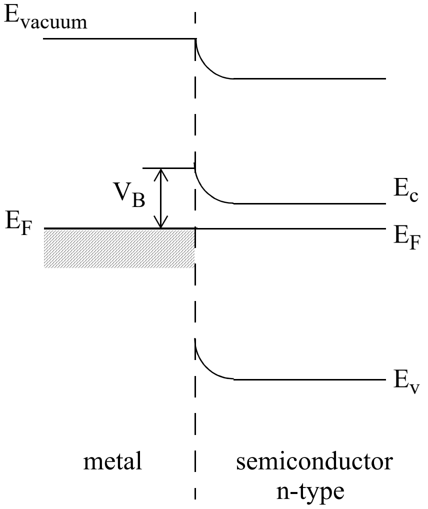
which means that significant errors in transit time may be induced by using the low field approximation in small semiconductor structures.

Problem 5

5.1

Metal semiconductor junction





This is a Schottky junction where electrons are depleted from the the metal semiconductor junction. The barrier height $V_B = \phi_m - \chi$ (metal workfunction - electron affinity).

5.2

A photon is absorbed by GaAs by creating an electron in the conduction band and a holde in the valence band. By using the reduced mass we may write

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

The energies of the electron and hole become

$$E_e - E_c = \frac{m_r^*}{m_e^*}(\hbar\omega - E_{gap}) = \frac{0{,}058}{0{,}067}(2 - 1{,}4) = 0{,}52eV$$

$$E_h - E_v = -\frac{m_r^*}{m_h^*}(\hbar\omega - E_{gap}) = \frac{-0{,}058}{0{,}45}(2 - 1{,}4) = -0{,}08eV$$

5.3

Using the contracted notation

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \dots & \sigma_{22} & \sigma_{23} \\ \dots & \dots & \sigma_{33} \end{bmatrix} = \begin{bmatrix} \sigma_1 & \sigma_6 & \sigma_5 \\ \dots & \sigma_2 & \sigma_4 \\ \dots & \dots & \sigma_3 \end{bmatrix}$$

we write

$$\begin{bmatrix} P_1 \\ P_2 \\ P_3 \end{bmatrix} = \begin{bmatrix} 2{,}3 & -2{,}3 & 0 & 0{,}67 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0{,}67 & -4{,}6 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix}$$

where the elements of the piezoelectric tensor is given in units of 10^{-12} C/N.

(a) Normal stress along the x-axis

$\sigma = \sigma_{11} = \sigma_1 = 2\cdot 10^4$ N/m^2 => $P_1 = 2.3\cdot 10^{-12} * 2\cdot 10^4$ C/m^2 = $4.6\cdot 10^{-8}$ C/m^2 , $P_2 = P_3 = 0$

(b) Shear stress around the x-axis

$\sigma = \sigma_{23} = \sigma_4 = 2\cdot 10^4$ N/m^2 => $P_1 = 0.67\cdot 10^{-12} * 2\cdot 10^4$ C/m^2 = $1.3\cdot 10^{-8}$ C/m^2 , $P_2 = P_3 = 0$