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:

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Date Signature

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

1.1 The carbon nano-tube transistor.....
A. has low thermal conductivity.
B. has low electrical conductivity.
C. has high electron mobility.
D. is easy to fabricate.

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

1.3 Topological insulators.....
A. are conducting in the bulk.
B. are conducting on the surface.
C. already have a range of applications.
D. are being used in quantum computers.

1.4 Si nano-wire transistors are.....
A. well suited for high-temperature applications.
B. promising for use in biosensor applications.
C. very costly to produce.
D. are relatively easy to downsize to below 10 nm.

1.5 Which statement is correct regarding optical data storage devices...
A. Magneto-optical storage devices are promising for storage of large amounts of data.
B. Longer optical wavelengths results in higher storage density.
C. Holographic methods show promise of improved data storage capabilities.
D. 5D data storage has been commercialized using fused silica.

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

1.7 Which statement regarding acousto-optic modulators (AOM) **is not** correct.....
A. AOMs may be used over a continuous range of wavelengths.
B. AOMs are used in laser applications.
C. The Bragg condition must be fulfilled in AOMs.
D. The theory of AOMs is well developed.

1.8 Piezoelectric transistors.....
A. may be made from centrosymmetric materials.
B. represent presently a mature technology.
C. may be based on PZT (lead zirconate titanate).
D. are slower than Si-based MOSFETs.

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

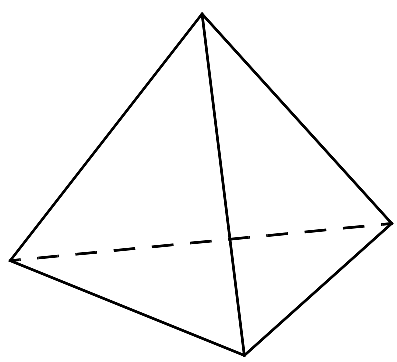
1.10 Which one of the following statements is correct:
A. a pyroelectric material is also ferroelectric
B. a ferroelectric material is also pyroelectric and piezoelectric
C. a piezoelectric material is also ferroelectric
D. the dielectric constant of a ferroelectric material is low

Problem 2

2.1 List the crystallographic symmetry operations.

2.2 Draw point group projections (stereograms) for the hexagonal point groups 32 and 622.

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



Problem 3

3.1

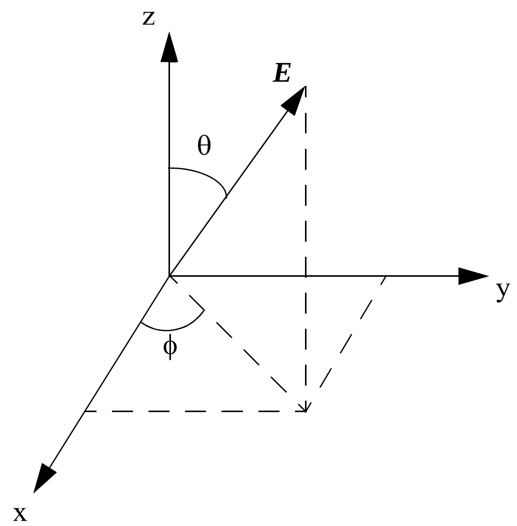
What is Neumann's principle?
Show how a two-fold rotational symmetry around the z-axis can be used to reduce the number of non-zero elements in a symmetric 2nd rank tensor.

3.2

Diagonalize a symmetric 2nd rank tensor of a monoclinic system by rotation around the z-axis.
Find an expression for the angle of rotation?

3.3

The electric field is pointing in a general direction as shown in the figure below.

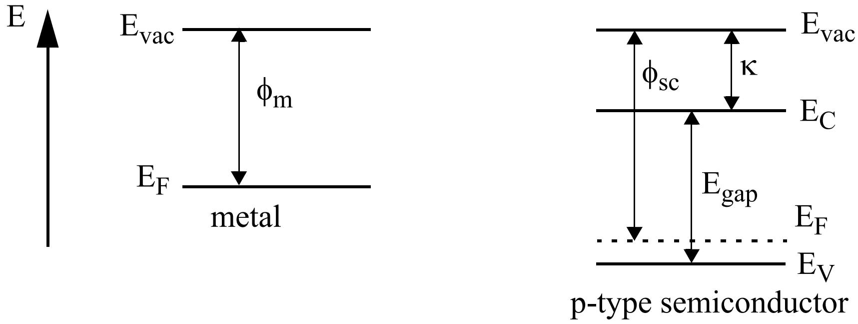


Find an expression for the magnitude of the dielectric permittivity in the direction of the electric field for an orthorhombic dielectric crystal.

Problem 4

4.1 Find the conductivity of a doped Si sample at a temperature of 300 K. The density of electrons in the conduction band is $n_d = 1 \cdot 10^{17}$ cm^{-3}. What is the conductivity due to the holes?

4.2 The figure below shows a schematic representation of the electronic levels in a metal and a p-doped semiconductor that are not in contact with each other. ϕ_m and ϕ_{sc} are the metal and semiconductor work functions, and κ is the electron affinity.



When the metal and semiconductor are placed in electrical contact the Fermi levels align.
Find the barrier height after contact has been made. What is this junction called?

4.3 Find the energy of the electron and hole (relative to the respective band edge) that results when a 1 eV photon is adsorbed by a germanium crystal having a band gap of 0.7 eV.

Problem 5

5.1 How should the biasing be for a pn-diode based opto-electronic device when used as a light detector? How should the biasing be for a light emitting pn-diode?

5.2 Name two crystallographic systems where uniaxial optical materials are to be found.
Also, name two crystallographic systems where biaxial optical materials may be found.

5.3 An electric field is applied in the z-direction of an electro-optic active cubic material. The index of refraction in the absence of an electric field is n_0. The influence of the electric field on the impermeability tensor is given by the Pockels effect:

$$\eta_{ij}(E) = \eta_{ij}^{0} + \sum_{k} r_{ijk} E_k$$

The material belongs to the crystallographic point group $\bar{4}3m$, and the only non-zero elements of the third rank tensor are r_{41}, r_{52} and r_{63} (using contracted notation). Write out the elements of the impermeability tensor.
What is the relation between the impermeability tensor and dielectric tensor?

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}, $\mu_n(Si) = 1000$ cm^2/Vs, $\mu_p(Si) = 350$ cm^2/Vs (low field values)

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

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

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 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:

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

Emission:

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

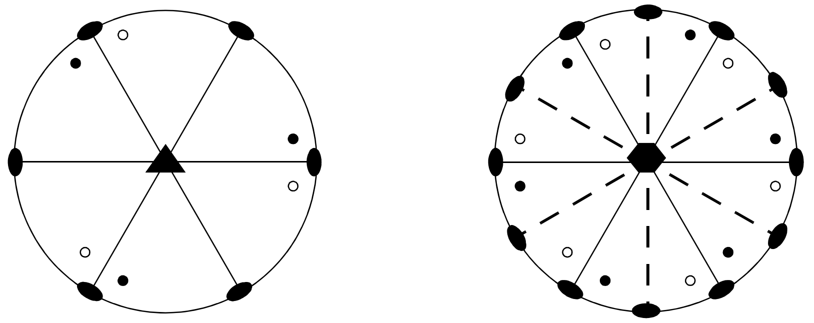
Solution Exam Dec.2, 2016.

Problem 1. Multiple choice questions: CABBC DACBB

Problem 2.

2.1. Identity, Inversion, Rotation, Reflection, Rotation-inversion

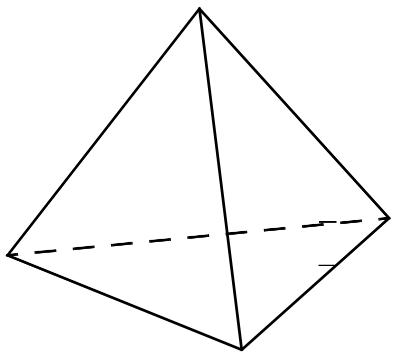
2.2. Stereograms



32 622

2.3.

Tetrahedron: 24 symmetry elements in the point group



1	- identity
m x 6	- mirror planes
2 x 3	- two-fold rotation
$3, 3^2$ x 4	- three-fold rotation
$\bar{4}, \bar{4}^3$	- four-fold rotation-inversion

(note that $\bar{4}^2$ = 2 two-fold rotation)

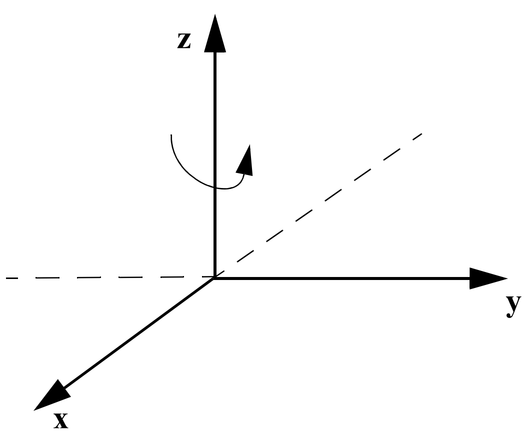
A total of 24 symmetry elements.

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.

Two-fold rotational symmetry reduces the number of non-zero elements in a second rank tensor: i



180^o rotation around the z-axis:

x' -> -x

y' -> -y

z' -> z

Since a second rank tensor ε transforms as the product of two coordinates we get:

$\varepsilon_{13} = -\varepsilon_{13}$

$\varepsilon_{23} = -\varepsilon_{23}$

Since this is a symmetry operation we must have that $\varepsilon_{ij}' = \varepsilon_{ij}$

which means that $\varepsilon_{13} = \varepsilon_{23} = 0$.

3.2

Will diagonalize a 2nd rank monoclinic tensor by rotation.

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

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

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

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

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

3.3

The components of the displacement vector may be written:

$$\varepsilon_E = D_E/E = \frac{\vec{D} \cdot \vec{E}}{E^2} = \sum_i D_i E_i / E^2 = \sum_{ij} \varepsilon_{ij} \left(\frac{E_j}{E}\right)\left(\frac{E_i}{E}\right)$$

From the figure we find:

$$x = E\sin\theta\cos\phi \qquad y = E\sin\theta\sin\phi \qquad z = E\cos\theta$$

For an orthorhombic only ε_{11}, ε_{22}, and ε_{33} are non-zero. Therefore we get:

$$\varepsilon_E = \varepsilon_{11}(\sin\theta\cos\phi)^2 + \varepsilon_{22}(\sin\theta\sin\phi)^2 + \varepsilon_{33}(\cos\theta)^2$$

Problem 4

4.1

The conductivity is given by

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

where the law of mass action has been used:

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

The hole conductivity is

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

4.2

The barrier height is given by: $E_B = \phi_m - \kappa - E_{gap}$

4.3

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

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

The energies of the electron and hole become

$$E_e - E_c = \frac{m_r^*}{m_e^*}(\hbar\omega - E_{gap}) = \frac{0{,}19}{0{,}56}(1 - 0{,}7) = 0{,}10 eV$$

$$E_h - E_v = -\frac{m_r^*}{m_h^*}(\hbar\omega - E_{gap}) = \frac{-0{,}19}{0{,}29}(1 - 0{,}7) = -0{,}20 eV$$

Problem 5

5.1
Reversed bias for a light detector, and forward bias for a light emitting diode.

5.2
Uniaxial optical materials: tetragonal, hexagonal, trigonal
Biaxial optical materials: orthorhombic, monoclinic, triclinic

5.3
The Pockels components of the impermeability tensor may be written:

$$\eta_{Pockels} = \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \\ \eta_5 \\ \eta_6 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ r_{41} & 0 & 0 \\ 0 & r_{52} & 0 \\ 0 & 0 & r_{63} \end{bmatrix} \cdot \begin{bmatrix} 0 \\ 0 \\ E \end{bmatrix}$$

This shows that only $\eta_6 = \eta_{12} = r_{63}E$ is non-zero.
Therefore:

$$\eta_{11} = \eta_1 = \frac{1}{n_0^2}$$

$$\eta_{22} = \eta_2 = \frac{1}{n_0^2}$$

$$\eta_{33} = \eta_3 = \frac{1}{n_0^2}$$

$$\eta_{12} = \eta_6 = r_{63} \cdot E \qquad others \qquad \eta_{ij} = 0$$

The relation between the impermeability and dielectric tensors:

$$\eta_{ij} = \frac{\varepsilon_0}{\varepsilon_{ij}}$$