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Department of Physics, NTNU

Examination paper for FY3114 Functional materials

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Examination date: December 4, 2018

Examination time (from-to): 9-13

Permitted examination support material:

Alternative C, Approved pocket calculator

K. Rottmann: Mathematical formulas (or equivalent)

English dictionary

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.

1 P1

Spintronics transistors....

Select one alternative

- ☐ demonstration devices exists
- ☐ use less power but are slower than ordinary transistors
- ☐ use the spin but not the charge of the electrons
- ☐ are already on the market

Graphene transistors....

Select one alternative

- ☐ well developed fabrication methods exist
- ☐ utilize high effective mass electrons
- ☐ have electron mobilities almost as high as in Si
- ☐ are candidates for even smaller electronic components

Organic semiconductor devices...

Select one alternative

- ☐ are well described theoretically
- ☐ are promising for display technologies
- ☐ possess a high degree of molecular orientation
- ☐ so far have high production costs

Which statement is correct?

- ☐ a ferroelectric material is also pyroelectric and piezoelectric
- ☐ a piezoelectric material is also ferroelectric
- ☐ the dielectric constant of a ferroelectric material is low
- ☐ a pyroelectric material is also ferroelectric

(1 point for each correct answer)

Maximum marks: 4

2 **P2**

Topological transistors....

Select one alternative:

- ☐ are conducting on the surface
- ☐ are conducting in the bulk
- ☐ are being used in quantum computation
- ☐ already have a wide range of applications

Piezoelectric transistors...

Select one alternative

- ☐ represent a mature technology
- ☐ may be used as strain sensors
- ☐ may be made from centrosymmetric materials
- ☐ are not suitable for use in touch devices

Si nanowire transistors....

Select one alternative

- ☐ provides less Joule heating
- ☐ have very small leakage currents
- ☐ only electrons carry the charge
- ☐ are relatively easy to fabricate

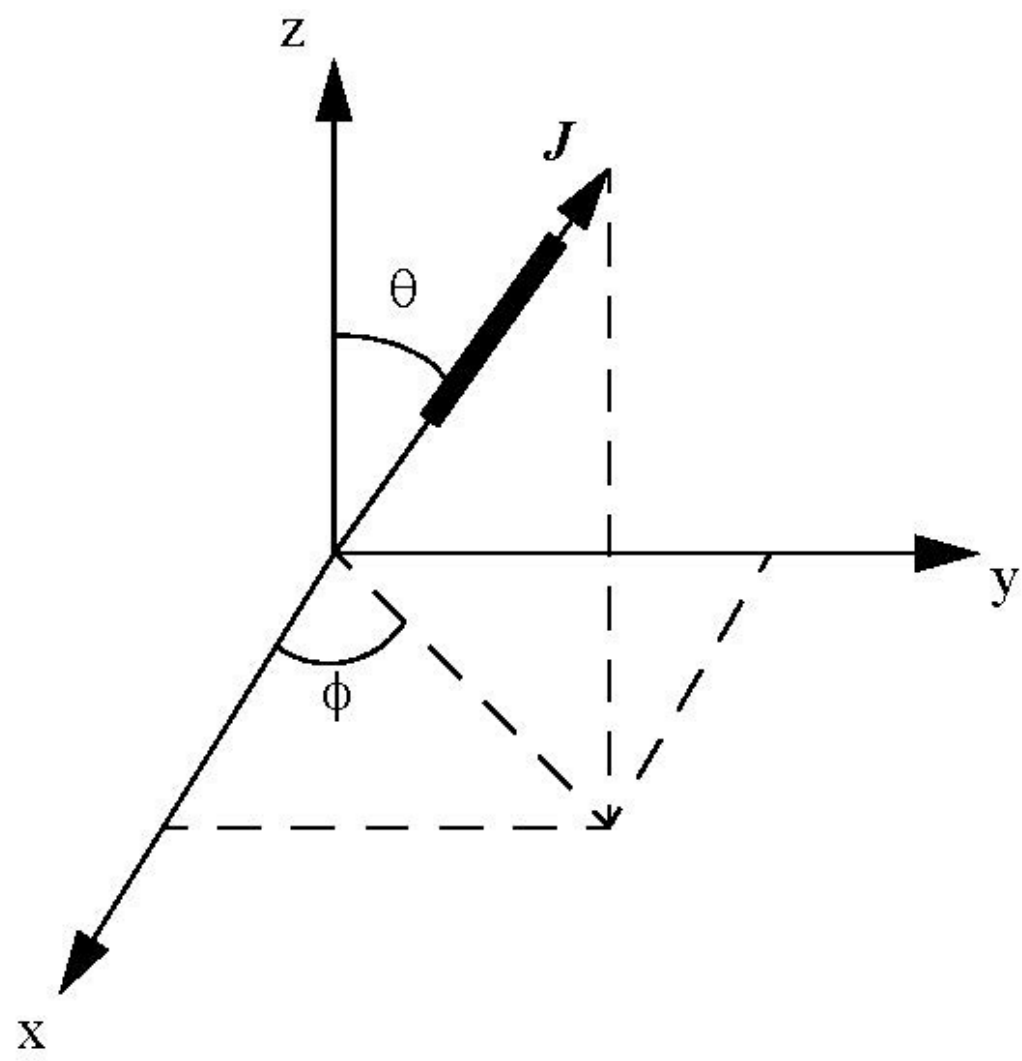
Which of the following crystal systems are uniaxial?

Select one alternative

- ☐ orthorombic
- ☐ cubic
- ☐ tetragonal
- ☐ monoclinic

(1 point for each correct answer)

3 P3



A trigonal conducting material is shaped as a long thin rod as shown in the figure above. The current density is $\mathbf{J}$. The rod is at an angle of $\theta = 30^\circ$ with the z-axis, and the projection of the rod in the xy-plane is at an angle $\phi = 45^\circ$ with the x-axis. Find the electrical resistivity along the direction of the rod in terms of the components of the resistivity tensor when $\rho_{11} = 8 \cdot 10^{-8} \Omega m$ and $\rho_{33} = 4 \cdot 10^{-8} \Omega m$.

Select one alternative:

- ☐ $3 \cdot 10^{-8} \Omega m$
- ☐ $4 \cdot 10^{-8} \Omega m$
- ☐ $5 \cdot 10^{-8} \Omega m$
- ☐ $6 \cdot 10^{-8} \Omega m$
- ☐ $8 \cdot 10^{-8} \Omega m$

(4 points for correct answer)

4 P4

Find the angle of rotation around the z-axis which diagonalize a symmetric 2nd rank tensor of a monoclinic system. The tensor elements are given to be $T_{11}=4$, $T_{22}=2$, and $T_{12}=1$.

Select one alternative:

- ☐ 22.5
- ☐ 33.4
- ☐ 45
- ☐ 30
- ☐ 42.2

The semiconductor InP has a band gap of 1.27 eV at room temperature (300 K). Find the energy of the electron and hole relative to the relevant band edges that results when a 1.5 eV photon is adsorbed.

The energy of the electron is:

Select one alternative

- ☐ 0.40 eV
- ☐ 0.20 eV
- ☐ 0.32 eV
- ☐ 0.15 eV
- ☐ 0.52 eV

The energy of the hole is:

Select one alternative

- ☐ -0.35 eV
- ☐ -0.034 eV
- ☐ -0.025 eV
- ☐ -0.15 eV
- ☐ -0.25 eV

(1 point for each correct answer)

Maximum marks: 3

5

P5

A p-doped Si sample is kept at temperature 300 K. The density of holes is $5 \cdot 10^{17} \text{ cm}^{-3}$. Use the law of mass action to find the conductivity due to the electrons.

The conductivity due to the electrons is:

Select one alternative

- ☐ $28.0 \frac{1}{\Omega \text{ cm}}$
- ☐ $3.6 \cdot 10^{-14} \frac{1}{\Omega \text{ cm}}$
- ☐ $14.0 \frac{1}{\Omega \text{ cm}}$
- ☐ $7.2 \cdot 10^{-14} \frac{1}{\Omega \text{ cm}}$
- ☐ $7.2 \cdot 10^{-12} \frac{1}{\Omega \text{ cm}}$

The conductivity due to the holes is:
Select one alternative

- ☐ $3.6 \cdot 10^{-14} \frac{1}{\Omega cm}$
- ☐ $28.0 \frac{1}{\Omega cm}$
- ☐ $7.2 \cdot 10^{-14} \frac{1}{\Omega cm}$
- ☐ $3.6 \cdot 10^{-14} \frac{1}{\Omega cm}$
- ☐ $14.0 \frac{1}{\Omega cm}$

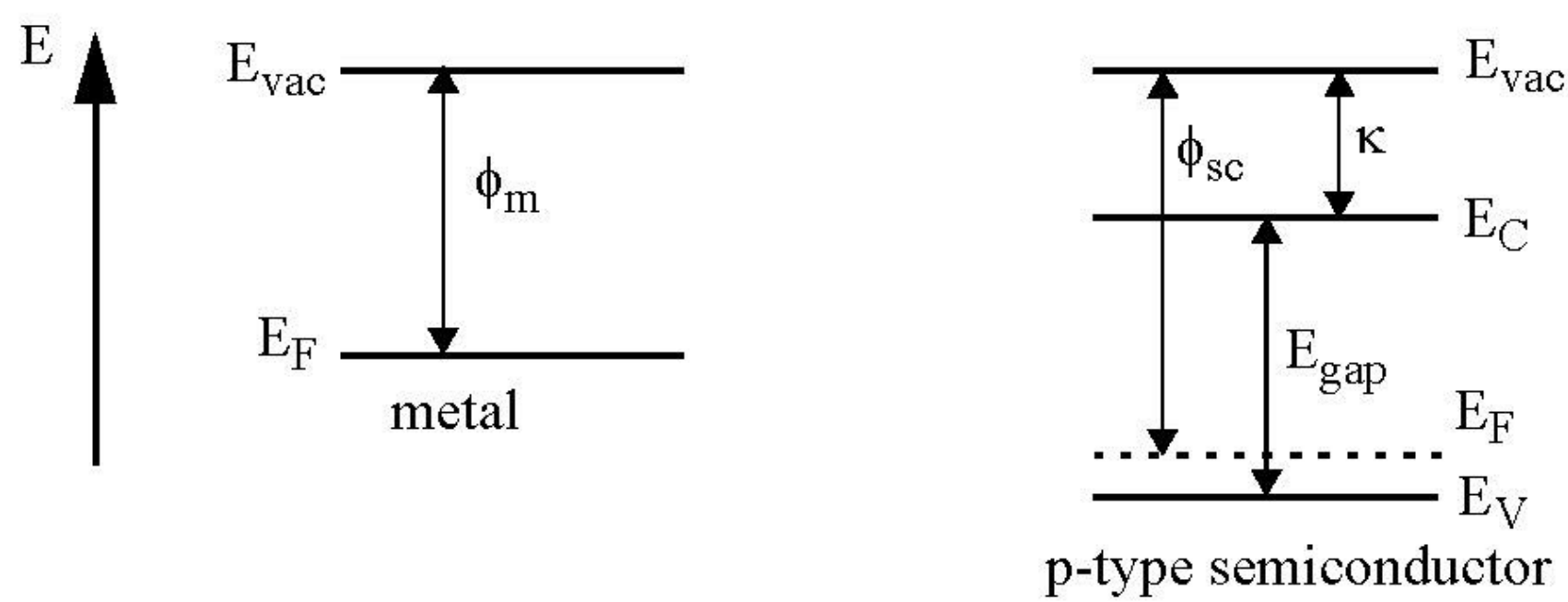
The conductivity of an undoped sample would be:
Select one alternative:

- ☐ $2.2 \cdot 10^{-6} \frac{1}{\Omega cm}$
- ☐ $2.6 \cdot 10^{-6} \frac{1}{\Omega cm}$
- ☐ $1.6 \cdot 10^{-6} \frac{1}{\Omega cm}$
- ☐ $3.2 \cdot 10^{-6} \frac{1}{\Omega cm}$
- ☐ $2.4 \cdot 10^{-6} \frac{1}{\Omega cm}$

(1 point for each correct answer)

Maximum marks: 3

6 P6



Schematic representations of the energy levels of a metal and a p-doped semiconductor are showed in the figure above. The work functions of metal and semiconductor are given by $\phi_M = 4.0$ and $\phi_{SC} = 4.8eV$; respectively. The energy gap of the semiconductor is $E_{gap} = 1.1eV$, and the electron affinity is $\kappa = 3.9eV$.
When the metal and semiconductor are contacted a Schottky junction forms.
The barrier height at the junction becomes:

- ☐ + 1.0 eV
- ☐ - 0.2 eV
- ☐ + 0.8 eV
- ☐ + 0.2 eV
- ☐ - 1.0 eV

(4 points for correct answer)

Maximum marks: 4

7

P7

Identify the stereograms (2D pointgroup projections) by placing the relevant point group notations on top of the stereograms (—4 means $\bar{4}$)

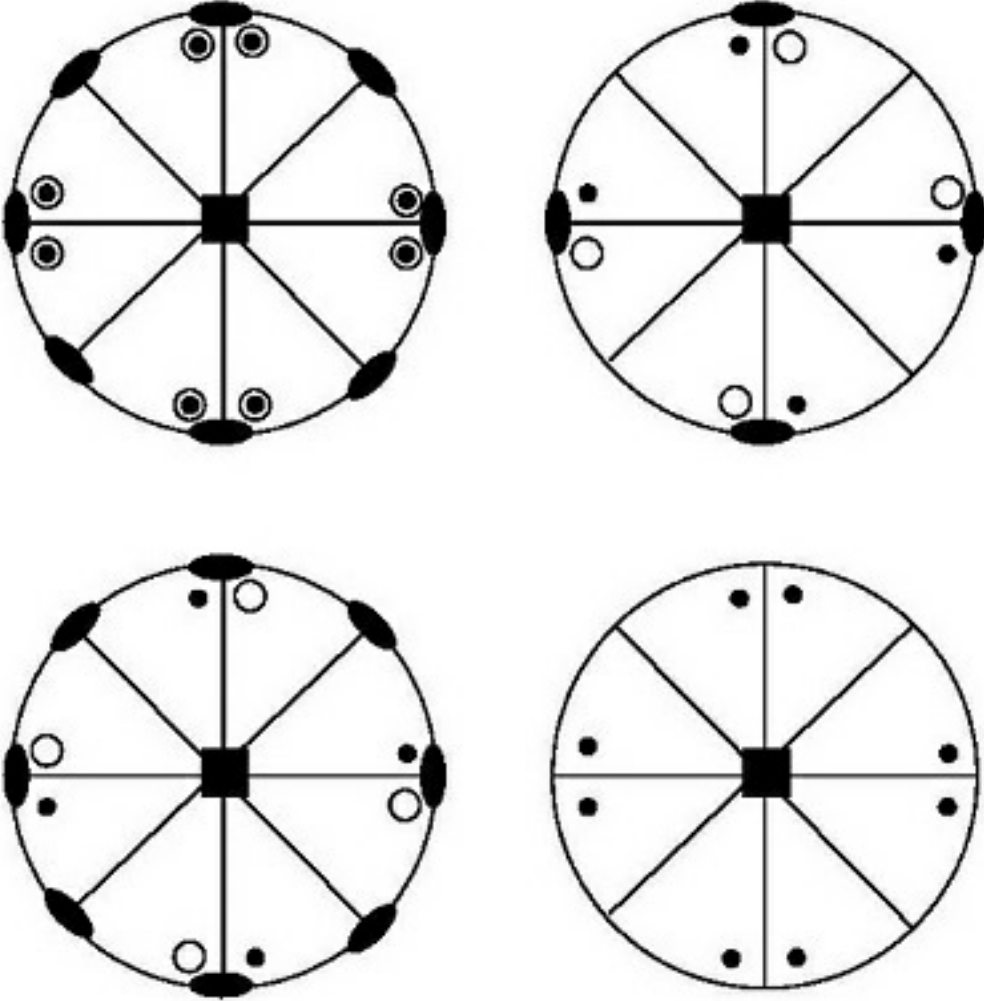
Move the point group notations listed on the left on top of the relevant stereogram

4mm

422

-42m

4/m 2/m 2/m



(1 point for each correct answer)

Maximum marks: 4

8

P8

Estimate the positions of the electron and hole quasi-Fermilevels (relative to the respective band edge) for Si at temperature 300 K when an electron density of $n = 4.5 \cdot 10^{17} \text{ cm}^{-3}$ and a hole density of $p = 2.2 \cdot 10^{17} \text{ cm}^{-3}$ are injected. Assume that $N_C = 2.8 \cdot 10^{19} \text{ cm}^{-3}$ and $N_V = 1.0 \cdot 10^{19} \text{ cm}^{-3}$.

The position of the electron quasi-Fermilevel is:

Select one alternative

- ☐ -0.11 eV
- ☐ -0.16 eV
- ☐ -0.32 eV
- ☐ -0.41 eV
- ☐ -0.20 eV

The position of the hole quasi-Fermilevel is:

Select one alternative

- ☐ 0.20 eV
- ☐ 0.17 eV
- ☐ 0.10 eV
- ☐ 0.42 eV
- ☐ 0.28 eV

(1 point for each correct answer)

Maximum marks: 2

9 P9

The piezoelectric tensor of of trigonal material of point group 32 is given by:

$$d = \begin{bmatrix} 3 & -3 & 0 & 5 & 0 & 0 \\ 0 & 0 & 0 & 0 & -5 & -6 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \text{ in units of } 10^{-12} C/N$$

The polarization along the x-axis for a normal stress $\sigma = 1 \cdot 10^4 Nm^{-2}$ along the y-axis is:

Select one alternative

- ☐ 0
- ☐ $-5 \cdot 10^{-8} Cm^{-2}$
- ☐ $-3 \cdot 10^{-8} Cm^{-2}$
- ☐ $3 \cdot 10^{-8} Cm^{-2}$
- ☐ $6 \cdot 10^{-8} Cm^{-2}$

The polarization along the y-axis for a shear stress $\sigma = 1 \cdot 10^4 Nm^{-2}$ around the z-axis is:

Select one alternative

- ☐ $-3 \cdot 10^{-8} Cm^{-2}$
- ☐ 0
- ☐ $5 \cdot 10^{-8} Cm^{-2}$
- ☐ $-6 \cdot 10^{-8} Cm^{-2}$
- ☐ $3 \cdot 10^{-8} Cm^{-2}$

The polarization along the y-axis for a shear stress $\sigma = 1 \cdot 10^4 Nm^{-2}$ around the y-axis is:

Select one alternative:

- ☐ 0
- ☐ $-3 \cdot 10^{-8} Cm^{-2}$
- ☐ $-6 \cdot 10^{-8} Cm^{-2}$
- ☐ $5 \cdot 10^{-8} Cm^{-2}$
- ☐ $-5 \cdot 10^{-8} Cm^{-2}$

(1 point for each correct answer)

Maximum marks: 3

10 P10

Soft ferromagnetic materials may be used for:

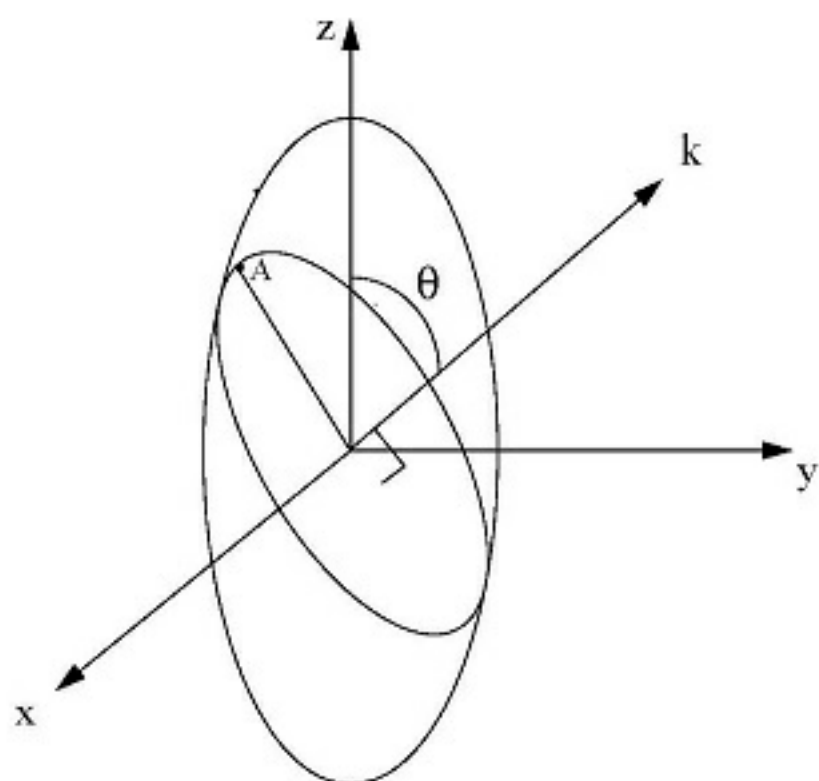
Select one or more alternatives:

- ☐ Magnetic recording devices
- ☐ Permanent magnets
- ☐ Magnetic shielding
- ☐ Motors
- ☐ Flux guides
- ☐ Transformers
- ☐ Induction ovens

(1 point for each correct answer)

Maximum marks: 3

11 P11



A uniaxial optical active material has index ellipsoid as shown above. The propagation direction of light is perpendicular to the ellipse shown in the figure, and the wave vector k is in the yz -plane. The point A is located on the ellipsoid and the ellipse in the yz -plane. The angle $\theta = 45^\circ$ and the ordinary and extraordinary indices of refraction are $n_{ro} = 1.6$ and $n_{re} = 1.5$.

What is the the refractive index $n_{re}(\theta)$ for light traveling in the k -direction?

- ☐ 1.51
- ☐ 1.53
- ☐ 1.55
- ☐ 1.57
- ☐ 1.59

(3 points for correct answer)

Maximum marks: 3

12

P12

Consider a Si pn-diode of area $A = 1\text{cm}^2$ that is used as a solar cell. The temperature is 300 K. The total current of the diode connected to an external load is given by $I = I_L - I_0(e^{eV/k_BT} - 1)$ where I_L is the photocurrent and I_0 is the diffusion current of electrons and holes. Find the open circuit ($I = 0$) voltage V_{OC} for the solar cell.

Parameter values are:

Density of electrons on the n-side: $n_n = 1 \cdot 10^{16}\text{cm}^{-3}$

Density of holes on the p-side: $p_p = 5 \cdot 10^{17}\text{cm}^{-3}$

Electron diffusion coefficient: $D_n = 20\text{cm}^2/s$

Hole diffusion coefficient: $D_p = 10\text{cm}^2/s$

Electron recombination time: $\tau_n = 3 \cdot 10^{-7}\text{s}$

Hole recombination time: $\tau_p = 1 \cdot 10^{-7}\text{s}$

Photocurrent: $I_L = 25\text{mA}$

The open circuit voltage V_{OC} is:

Select one alternative:

- ☐ 0.67 V
- ☐ 0.32 V
- ☐ 0.44 V
- ☐ 0.53 V
- ☐ 0.25 V

(3 points for correct answer)

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- ☐ are well described theoretically
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Which statement is correct?

Select one alternative

- ☐ the dielectric constant of a ferroelectric material is low
- ☒ a ferroelectric material is also pyroelectric and piezoelectric
- ☐ a pyroelectric material is also ferroelectric
- ☐ a piezoelectric material is also ferroelectric

(1 point for each correct answer)

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2 P2

Topological transistors....

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Which of the following crystal systems are uniaxial?

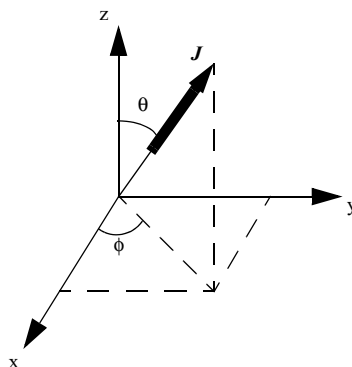
Select one alternative

- ☒ tetragonal
- ☐ cubic
- ☐ orthorombic
- ☐ monoclinic

(1 point for each correct answer)

Solution Exam Dec.4, 2018.**Problem 1.** Project relevant questions: xxxx**Problem 2.** Project relevant questions: xxxx**Problem 3**

A trigonal conducting material is shaped as a long thin rod, and is directed as shown in the figure below. The current $\mathbf{J}$ 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 $\mathbf{J}$ in terms of the components of the resistivity tensor.



The resistivity tensor of a trigonal solid is given by

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

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

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

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

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

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

$$\begin{aligned} \rho_J &= \rho_{11} (\sin \theta \cos \phi)^2 + \rho_{11} (\sin \theta \sin \phi)^2 + \rho_{33} (\cos \theta)^2 \\ \rho_J &= \rho_{11} \left(\frac{1}{2} \frac{1}{\sqrt{2}} \right)^2 + \rho_{11} \left(\frac{1}{2} \frac{1}{\sqrt{2}} \right)^2 + \rho_{33} \left(\frac{\sqrt{3}}{2} \right)^2 = \frac{\rho_{11}}{4} + \frac{3\rho_{33}}{4} \end{aligned}$$

Problem 4

Find the angle of rotation around the z-axis which diagonalize a symmetric 2nd rank tensor of a monoclinic system. The tensor elements are given to be $T_{11}=4$, $T_{22}=2$, and $T_{12}=1$.

Will diagonalize a 2nd rank monoclinic tensor by rotation.

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

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

$$\text{and} \quad T_{12} = (T_{22} - T_{11}) \frac{\sin 2\theta}{2} + T_{12} \cos 2\theta$$

For $T'_{12} = 0$ we get:

$$\tan 2\theta = \frac{2T_{12}}{T_{11} - T_{22}} = 1 \Rightarrow \theta = 22,5^\circ$$

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.

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

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

The energies of the electron and hole become

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

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

Problem 5

A p-doped Si sample is at a temperature of 300 K. The density of holes in the valence band is $p_a = 5 \cdot 10^{17} \text{ cm}^{-3}$. 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.

The conductivity is given by

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

where the law of mass action has been used:

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

The conductivities are

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

Problem 6

Schematic representations of the energy levels of a metal and a p-doped semiconductor are showed in the figure. The work functions of metal and semiconductor are given by 4.0 and 4.8 eV; respectively. The energy gap of the semiconductor is 1.1 eV, and the electron affinity is 3.9 eV. When the metal and semiconductor are contacted a Schottky junction forms. The barrier height at the junction becomes: $V_b = 4.0 - 1.1 - 3.9 = -1.0 \text{ eV}$

Problem 7

See table of stereograms for the 32 crystallographic point groups.

Problem 8

Estimate the positions of the electron and hole quasi-Fermilevels (relative to the respective band edge) for Si at temperature 300 K when an electron density of $n=4.5 \cdot 10^{17} \text{ cm}^{-3}$ and a hole density of $p=2.2 \cdot 10^{17} \text{ cm}^{-3}$ are injected. Assume that $N_C=2.8 \cdot 10^{19} \text{ cm}^{-3}$ and $N_V=1.0 \cdot 10^{19} \text{ cm}^{-3}$.

$$E_{Fn} - E_C = k_B T \cdot \ln \frac{n}{N_C} = -0,11 \text{ eV}$$

$$E_{Fp} - E_V = -k_B T \cdot \ln \frac{p}{N_V} = 0,10 \text{ eV}$$

Problem 9

The piezoelectric tensor of a trigonal material of point group 32 is given by:

$$d = \begin{bmatrix} 3 & -3 & 0 & 5 & 0 & 0 \\ 0 & 0 & 0 & 0 & -5 & -6 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

in units of 10^{-12} C/N .

The polarization along the the x-axis for normal stress $\sigma = 10^4 \text{ Nm}^{-2}$ along the y-axis:

$$P_1 = d_{12} \sigma = -3 \cdot 10^8 \text{ Cm}^{-2}$$

The polarization along the the y-axis for shear stress $\sigma = 10^4 \text{ Nm}^{-2}$ around the z-axis:

$$P_1 = d_{12} \sigma = -6 \cdot 10^8 \text{ Cm}^{-2}$$

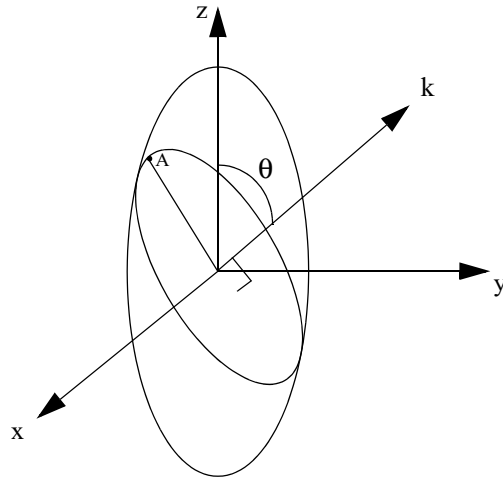
The polarization along the the y-axis for shear stress $\sigma = 10^4 \text{ Nm}^{-2}$ around the y-axis:

$$P_1 = d_{12} \sigma = -5 \cdot 10^8 \text{ Cm}^{-2}$$

Problem 10

Soft ferromagnetic materials may be used for: transformers, flux guides and magnetic shielding.

Problem 11



A uniaxial optical active material has index ellipsoid as shown above. The propagation direction of light is perpendicular to the ellipse shown in the figure, and the wave vector k is in the yz -plane. The point A is located on the ellipsoid and the ellipse in the yz -plane. The angle $\theta=45^\circ$ and the ordinary and extraordinary indices of refraction are $n_{ro}=1.6$ and $n_{re}=1.5$. What is the refractive index $n_{re}(\theta)$ for light traveling in the k -direction?

From figure: $x_A = 0$, $y_A = |A|\cos\theta$, $z_A = |A|\sin\theta$

From ellipse: $|A| = n_{re}(\theta)$

The point A is on the index ellipsoid:

$$\frac{x_A^2}{n_{ro}^2} + \frac{y_A^2}{n_{ro}^2} + \frac{z_A^2}{n_{re}^2} = 1 \Rightarrow \frac{n_{re}(\theta) \cdot (\cos\theta)^2}{n_{ro}^2} + \frac{n_{re}(\theta) \cdot (\sin\theta)^2}{n_{re}^2} = 1$$

and we get:

$$\frac{1}{n_{re}(\theta)^2} = \frac{(\cos\theta)^2}{n_{ro}^2} + \frac{(\sin\theta)^2}{n_{re}^2}$$

Inserting numbers gives: $n_{re}(\theta=45^\circ) = 1.55$

Problem 12

Consider a Si pn-diode that is used as a solar cell. The temperature is 300 K. The total current of the diode connected to an external load is given by I where I_L is the photocurrent and I_0 is the diffusion current of electrons and holes. Find the open circuit voltage for the solar cell.

$$I = I_L - I_0(e^{eV/k_B T} - 1)$$

Diffusion currents for electrons on the p-side and holes on the n-side is:

$$J_n = eD_n \frac{dn}{dx} = eD_n \cdot \frac{n_p}{L_n} \quad \text{and} \quad J_p = eD_p \frac{dp}{dx} = eD_p \cdot \frac{p_n}{L_p}$$

Therefore:

$$\frac{I_0}{A} = eD_n \cdot \frac{n_p}{L_n} + eD_p \cdot \frac{p_n}{L_p} \quad \text{where} \quad L_n = \sqrt{D_n \tau_n} \quad \text{and} \quad L_p = \sqrt{D_p \tau_p}$$

The open circuit voltage becomes ($I=0$):

$$V_{OC} = \frac{k_B T}{e} \ln\left(1 + \frac{I_L}{I_0}\right) = 0,53 \text{ V}$$