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Department of physics

Examination paper for FY3114 Functional Materials

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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 Which of these properties charcterizes a carbon nano-tube transistor?
- **A.** Low effective electron mass.
- **B.** High electron mobility.
- **C.** Low thermal conductivity.
- **D.** Easy to fabricate.

1.2 Which of the following statements does not apply to 3-5 compound nanowire transistors?
- **A.** The bandgap may be controlled.
- **B.** High electron mobility.
- **C.** Low surface/volume ratio.
- **D.** Low power consumption.

1.3 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.

1.4 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.

1.5 Which statement is wrong regarding materials used for optical data storage?
- **A.** Magneto-optical storage devices rely on light rare earth based magnets.
- **B.** Longer optical wavelengths results in higher storage density.
- **C.** Holographic methods show promise of improved data storage capabilities.
- **D.** Thinner active layers on discs are required for improved storage.

1.6 Organic semiconductor devices are characterized by:
- **A.** Being promising in display technologies.
- **B.** High production costs.
- **C.** High molecular orientation.
- **D.** Good theoretical understanding.

1.7 Si nano-wire transistors are:
- **A.** characterized by low leakage currents.
- **B.** not dependent on quantum effects.
- **C.** hampered by low speed capabilities.
- **D.** promising for use in biosensor applications.

1.8 High T_c superconductors:
A. may be explained by the BCS theory
B. may be ferromagnetic
C. may possibly be used in quantum computing
D. have reached critical temperatures of above 200 K

1.9 The spintronic transistor:
A. has already been fabricated
B. relies on spin polarized electrons
C. may not be made from Si
D. must include paramagnetic contacts

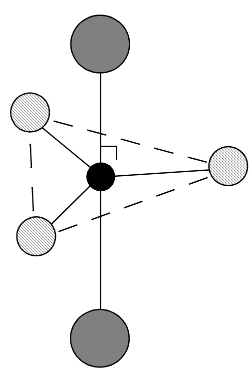
1.10 Which of the following crystal systems is uniaxial?:
A. cubic
B. tetragonal
C. orthorombic
D. monoclinic

Problem 2

2.1 Explain why polar point groups cannot contain an inversion centre.

2.2 Draw point group projections (stereograms) for the tetragonal point groups 4 and 4mm.

2.3 How many symmetry elements is contained in the point group of the PF_3Cl_2 molecule as shown below? The plane containing the three F atoms is perpendicular to the axis between the Cl atoms.
List these symmetry elements.



Problem 3

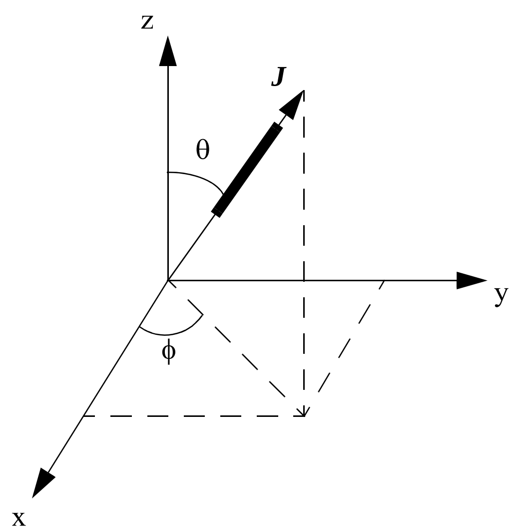
3.1

Explain briefly the difference between intrinsic and point group symmetry of an anisotropic material. State Neumann's principle.

3.2

Draw a cube and indicate the normal and shear stresses on the faces of the cube.
Show that the stress tensor is symmetric for materials in static equilibrium (using the drawing).

3.3



A thin rod of a monoclinic conducting material is directed as shown in the figure.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. The current $\boldsymbol{J}$ flows in the direction of the rod.

Find the electrical resistivity ρ_J along the direction of the current $\boldsymbol{J}$ in terms of the components of the resistivity tensor..

Problem 4

4.1 Calculate the scattering relaxation time for electrons in pure GaAs at a temperture of 300 K. When the sample is n-doped at $N_d = 1 \cdot 10^{17}$ cm^{-3} the mobility decreases to 5000 cm^2/Vs. Assume that the total scattering rate is the sum of scattering rates of the pure sample and the scattering rate due to impurities and calculate the scattering relaxation time due to impurities.

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

4.3 Calculate the transit time for an electron through a GaAs device of dimension 1 μm by using the low field approximation. The electric field across the device is 5 kV/cm.
Is the low field approximation valid in this case?

Problem 5

5.1 Estimate the position of the electron and hole quasi-Fermilevels (relative to the respective band edge) for Si at a temperature of 300 K when an electron and hole density $n = p = 1 \cdot 10^{17}$ cm^{-3} is injected. Assume that $N_c = 2.8 \cdot 10^{19}$ cm^{-3} and $N_v = 1.0 \cdot 10^{19}$ cm^{-3} at T = 300 K.

5.2 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.

5.3 The Piezoelectric tensor of the tetragonal material PZT-5H (point group 4mm) is given by:

$$d = \begin{bmatrix} 0 & 0 & 0 & 0 & 735 & 0 \\ 0 & 0 & 0 & 735 & 0 & 0 \\ -263 & -263 & 515 & 0 & 0 & 0 \end{bmatrix}$$

in units of 10^{-12} C/N. Calculate the polarization along x, y and z axes for:
(a) Shear stress $\sigma = 1 \cdot 10^4$ N/m^2 around the x-axis.
(b) Shear stress $\sigma = 1 \cdot 10^4$ N/m^2 around the y-axis.
(c) Normal stress $\sigma = 1 \cdot 10^4$ N/m^2 along the z-axis.

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:

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

Magnitude of $\boldsymbol{D}$ along $\boldsymbol{E}$:

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

Dielectric permittivity tensor:

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

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

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:

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

Emission:

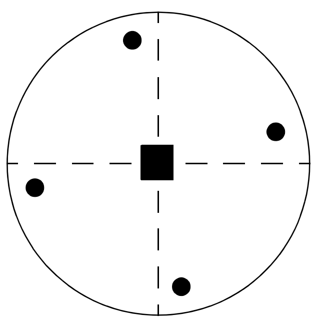
$$\hbar\omega = E_e - E_h = E_{gap} + \frac{(\hbar k)^2}{2m_r^*} \qquad W_{em}^{st}(\hbar\omega) = \frac{e^2 n_r \hbar\omega}{3\pi\varepsilon_0 m_e^2 c^3 \hbar^2}|p_{cv}|^2 \cdot n_{ph}(\hbar\omega) \qquad \frac{2|p_{cv}|^2}{m_e} = 23eV \quad (GaAs)$$

Problem 1. Multiple choice questions: BCCBB ADCBB

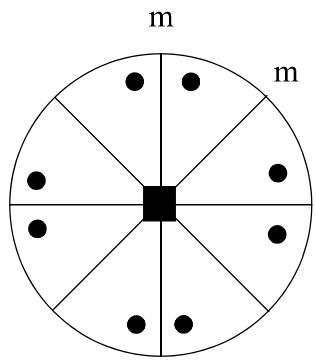
Problem 2.

2.1. We must require that the components of a vector are invariant under symmetry operations, and therefore the presence of an inversion centre prohibits vector properties since **P** -> -**P**.

2.2. Stereograms

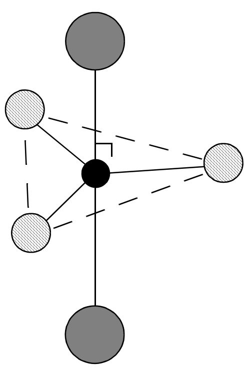


4



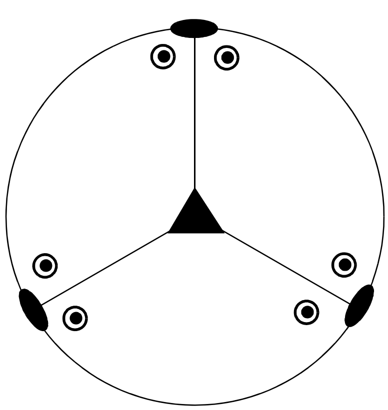
4mm

2.3.
PF_3Cl_2 molecule



1	- identity
m,m,m	- mirror planes
1/m	- mirror plane (vertical)
2,2,2	- 2-fold rotatiom
$3, 3^2$	- 3-fold rotation
$\overline{6}$	- 6-fold rotation-inversion
$\overline{6}^5$	- five times 6-fold rotation-inversion

A total of 12 symmetry elements.



Stereogram for the PF_3Cl_2 molecule showing 12 GEP (General Equivalent Points)

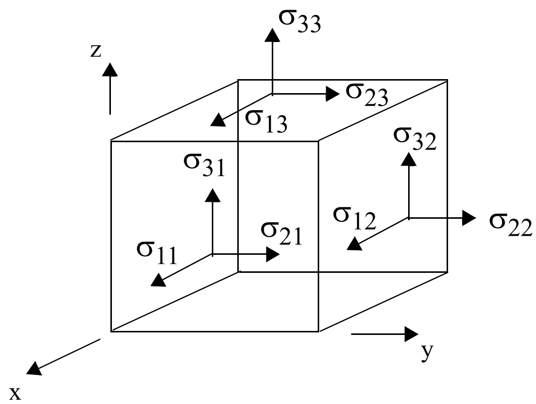
Problem 3

3.1

Instrinsic symmetry is caused by physical contraints.

Neumann's principle states that a physical property of an anisotropic material must at least possess the symmetry of the crystallographic point group.

3.2



Normal stresses σ_{11}, σ_{22} and σ_{33}. The others are shear stresses.

If the cube is in static equilibrium (not rotating) we must have that $\sigma_{31} = \sigma_{13}$ etc.

3.3

The resistivity tensor of a monoclinic solid is given by

$$\rho_{monoclinic} = \begin{bmatrix} \rho_{11} & \rho_{12} & 0 \\ \rho_{12} & \rho_{22} & 0 \\ 0 & 0 & \rho_{33} \end{bmatrix} \quad and \quad \begin{bmatrix} E_1 \\ E_2 \\ E_3 \end{bmatrix} = \begin{bmatrix} \rho_{11} & \rho_{12} & 0 \\ \rho_{12} & \rho_{22} & 0 \\ 0 & 0 & \rho_{33} \end{bmatrix} \begin{bmatrix} J_1 \\ J_2 \\ J_3 \end{bmatrix}$$

The resisitivity along 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

$$\rho_J = \rho_{11}\left(\frac{J_x}{J}\right)^2 + \rho_{22}\left(\frac{J_y}{J}\right)^2 + \rho_{33}\left(\frac{J_z}{J}\right)^2 + 2\rho_{12}\left(\frac{J_x}{J}\right)\left(\frac{J_y}{J}\right)$$

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 $\phi = 45^o$

$$\rho_J = \rho_{11}(\sin\theta\cos\phi)^2 + \rho_{22}(\sin\theta\sin\phi)^2 + \rho_{33}(\cos\theta)^2 + 2\rho_{12}(\sin\theta)^2(\sin\phi\cos\phi)$$

$$\rho_J = \rho_{11}\left(\frac{1}{2}\frac{1}{\sqrt{2}}\right)^2 + \rho_{22}\left(\frac{1}{2}\frac{1}{\sqrt{2}}\right)^2 + \rho_{33}\left(\frac{\sqrt{3}}{2}\right)^2 + 2\rho_{12}\left(\frac{1}{2}\right)^2\left(\frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\right) = \frac{\rho_{11}}{8} + \frac{\rho_{22}}{8} + \frac{3\rho_{33}}{4} + \frac{\rho_{12}}{4}$$

Problem 4

4.1

The scattering rate may be found from and the numbers from page 6:

$$\mu_n = e\tau_{sc}/m^* \quad \Rightarrow \quad \tau_{sc} = \frac{m^*\mu_n}{e} = 3{,}05 \cdot 10^{-13} s$$

the scattering rates are related as

$$r_{doped} = r_{intrinsic} + r_{impurity} \quad \Rightarrow \quad \frac{1}{\tau_{doped}} = \frac{1}{\tau_{sc}} + \frac{1}{\tau_{impurity}} = \frac{e}{m^*\mu_{doped}} = 5{,}25 \cdot 10^{12}$$

the impurity scattering relaxation time becomes

$$\frac{1}{\tau_{impurity}} = \frac{e}{m^*\mu_{doped}} - \frac{1}{\tau_{sc}} = 1{,}97 \cdot 10^{12}\frac{1}{s} \quad \Rightarrow \quad \tau_{impurity} = 5{,}1 \cdot 10^{-13} s$$

4.2

The conductivity is given by

$$\sigma = \sigma_n + \sigma_p = ne\mu_n + pe\mu_p = n_d e\mu_n + \frac{n_i^2}{n_d}e\mu_p = 128\frac{1}{\Omega cm} + 2{,}2 \cdot 10^{-21}\frac{1}{\Omega cm} = 128\frac{1}{\Omega cm}$$

where the law of mass action has been used:

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

The hole conductivity is

$$\sigma_p = 2{,}2 \cdot 10^{-21}\frac{1}{\Omega cm}$$

4.3

The transit time through the device is given by

$$t = \frac{L}{v_d} \qquad and \qquad \mathbf{v_d}(lowfield) = \mu_n E = 8000 \cdot 5000\frac{cm}{s} = 4 \cdot 10^7\frac{cm}{s}$$

therefore

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

The low field approximation is not a good approximation since the calculated drift velocity of the electron exceeds the saturation value of about $1 \cdot 10^7$ cm/s.

Problem 5

5.1

The positions of the quasi-Fermilevels may be estimated from:

$$n = N_c e^{-(E_c - E_{Fn})/k_B T} \quad and \quad p = N_v e^{-(E_{Fp} - E_v)/k_B T}$$

which gives

$$E_{Fn} - E_c = k_B T \cdot \ln\left(\frac{n}{N_c}\right) = -2{,}3 \cdot 10^{-20} J = -0{,}15 eV$$

$$E_{Fp} - E_v = -k_B T \cdot \ln\left(\frac{p}{N_v}\right) = 1{,}9 \cdot 10^{-20} J = 0{,}12 eV$$

5.2

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

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

The energies of the electron and hole become

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

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

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

$$\begin{bmatrix} P_1 \\ P_2 \\ P_3 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & 735 & 0 \\ 0 & 0 & 0 & 735 & 0 & 0 \\ -263 & -263 & 515 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix}$$

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

(a) Shear stress around the x-axis

$\sigma = \sigma_{23} = \sigma_4 = 1 \cdot 10^4$ N/m^2 => $P_2 = 735 \cdot 10^{-12} * 1 \cdot 10^4$ C/m^2 = $7.35 \cdot 10^{-6}$ C/m^2 , $P_1 = P_3 = 0$

(b) Shear stress around the y-axis

$\sigma = \sigma_{13} = \sigma_5 = 1 \cdot 10^4$ N/m^2 => $P_1 = 735 \cdot 10^{-12} * 1 \cdot 10^4$ C/m^2 = $7.35 \cdot 10^{-6}$ C/m^2 , $P_2 = P_3 = 0$

(c) Normal stress along the z-axis

$\sigma = \sigma_{33} = \sigma_3 = 1 \cdot 10^4$ N/m^2 => $P_3 = 515 \cdot 10^{-12} * 1 \cdot 10^4$ C/m^2 = $5.15 \cdot 10^{-6}$ C/m^2 , $P_1 = P_2 = 0$