

School of Computing, Science & Engineering

SEMESTER TWO EXAMINATION

PROGRAMMES:

MPhys Physics

MPhys Physics with studies in North America

BLOCK CODES:

MP/P/F4 MP/PN/F4 MP/PAT/F4

MP/P/S5 MP/PAT/S5

THIN FILMS AND MATERIALS CHARACTERISATION P1

Tuesday 17 May 2016

14:00 – 17:00

Instructions to Candidates

Time allowed 3 hours

Answer the question in **SECTION A** **AND** any **THREE** questions from **SECTION B**

The question in Section A carries 40 marks. Each question in Section B carries 20 marks.

You are advised to spend 70 minutes on Section A and 36 minutes on each question in Section B.

Standard List of Physical Constants is provided.

Approved electronic calculators may be used.

STANDARD LIST OF PHYSICAL CONSTANTS

Acceleration due to gravity,	g	=	9.81 m s^{-2}
Atomic mass unit,	u	=	$1.66 \times 10^{-27} \text{ kg}$
Avogadro constant,	N	=	$6.02 \times 10^{23} \text{ mol}^{-1}$
Bohr magneton,	μ_B	=	$9.27 \times 10^{-24} \text{ J T}^{-1}$
Boltzmann constant,	k_B	=	$1.38 \times 10^{-23} \text{ J K}^{-1}$
Electron charge,	e	=	$1.60 \times 10^{-19} \text{ C}$
Electron rest mass,	m_e	=	$9.11 \times 10^{-31} \text{ kg}$
Faraday constant,	F	=	$9.65 \times 10^4 \text{ C mol}^{-1}$
Gas constant,	R	=	$8.3 \text{ J mol}^{-1} \text{ K}^{-1}$
Gravitational constant,	G	=	$6.672 \times 10^{-11} \text{ N m}^2 \text{ kg}^{-2}$
Permeability of free space,	μ_0	=	$4\pi \times 10^{-7} \text{ H m}^{-1}$
Permittivity of free space,	ϵ_0	=	$8.85 \times 10^{-12} \text{ F m}^{-1}$
Planck constant,	h	=	$6.63 \times 10^{-34} \text{ J s}$
Proton rest mass,	m_p	=	$1.67 \times 10^{-27} \text{ kg}$
Rydberg constant,	R_∞	=	$1.0974 \times 10^7 \text{ m}^{-1}$
Solar constant	S_0	=	$1.37 \times 10^3 \text{ W m}^{-2}$
Stefan-Boltzmann constant	σ	=	$5.670 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$
Velocity of light in vacuo,	c	=	$3.00 \times 10^8 \text{ m s}^{-1}$
	1 eV	=	$1.60 \times 10^{-19} \text{ J}$

SECTION A

1. Answer **ALL** parts of the question:

(a) Why is lattice matching important in the deposition of high quality epitaxial semiconductor thin films? Include an example of a thin film and its properties which are affected by lattice matching. (4 marks)

(b) Explain why interference fringe colours are seen for thin films, but not for bulk materials. (3 marks)

(c) Draw a schematic diagram of a *Molecular Beam Epitaxy* coater. Briefly explain the basic functions of key components. (4 marks)

(d) State four advantages of using the atmospheric pressure *chemical vapour deposition* process (APCVD) over that of physical vacuum techniques. (2 marks)

(e) Name two factors that could affect the resolution of the scanning electron microscope (SEM). (1 mark)

(f) The image generated by an SEM is displayed on a screen of dimensions 200 mm × 200 mm. If the image contains 1000 raster lines and the instrument is operating at a magnification of 10,000×, what is the ideal probe size on the specimen? (2 marks)

(g) An SEM is operating such that 5×10^4 electrons fall upon each element (pixel) of sample area. If the total raster time is 5 seconds and the number of raster lines is 1000, estimate the absolute current of the incident electron probe. (2 marks)

(h) What are the two principal techniques used for the collection of X-ray data in analytical *electron microscopy*? Give an advantage and disadvantage of each method. (2 marks)

(i) Briefly explain the *Auger process* in atoms. Draw schematic diagrams to illustrate the initial and final states of an Auger process. (3 marks)

(j) What is the main difference between a *second* and a *third* generation synchrotron? Draw a schematic diagram for the *storage ring* of a third generation synchrotron, annotate the key components and briefly explain their functions.

(3 marks)

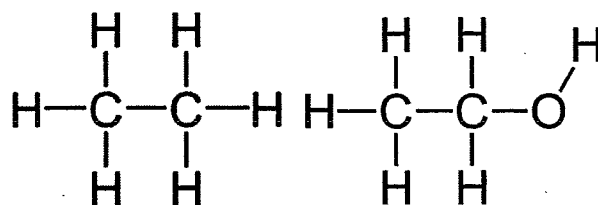
(k) Briefly explain the difference between *ionic* and *covalent* bonding.

(4 marks)

(l) How many lattice points can the primitive unit cell of a crystal contain? How many atoms can the primitive unit cell of a crystal contain?

(4 marks)

(m) Do the ethane and ethanol molecules (sketched below) have a permanent electric dipole moment? If not, can an electric dipole moment be induced if the molecule is vibrating?



Ethane

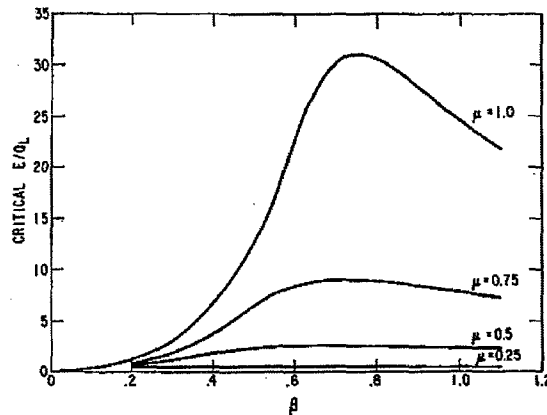
Ethanol

(6 marks)

SECTION B

2.

(a) One of the stages of film formation is *thermal accommodation*. Within this stage a 1D harmonic oscillator model has been used to describe how energy is transferred to the substrate lattice, resulting in the diagram below.

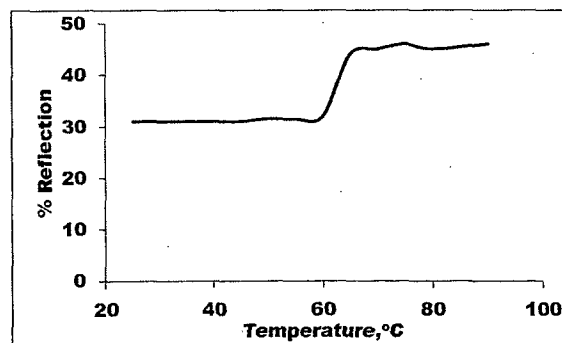


Define the symbols used in the diagram and explain:

- (i) the physical importance of the area under the curve;
- (ii) the relationship between E/Q_L and μ ;
- (iii) the relationship between E/Q_L and β (over the range 0 to 0.75).

(8 marks)

(b) Vanadium dioxide, VO_2 is thermochromic, changing at a critical temperature T_c from semiconductor (refractive index, $n=3$) to metal ($n=1.1$). Thin films of VO_2 and titanium oxide, TiO_2 ($n=2.5$) are deposited on a glass substrate with the VO_2 as the upper layer. The diagram below shows the effect of temperature on optical reflection for this sample. Considering your knowledge of the behaviour of light relative to the refractive index at the different interfaces, give an explanation of why at the critical transition temperature the reflection increases?



(4 marks)

QUESTION 2 IS CONTINUED ON THE NEXT PAGE...

(c) Discuss the chemical, kinetic and mass transport behaviour in CVD with particular reference to the deposition temperature 'volcano curve'.

(5 marks)

(d) Molybdenum is vacuum evaporated from a point source onto a circular substrate of 1.5 cm diameter placed directly above the source. The rate of molybdenum evaporation is constant at $2.3 \times 10^{-8} \text{ kg s}^{-1}$, the percentage of evaporated molybdenum reaching the substrate is 3% and the sticking coefficient at the substrate is 0.4. After deposition lasting 2 minutes the deposited film is found to be of uniform thickness 200 nm. Calculate the film density as a percentage of the bulk density of molybdenum ($1.019 \times 10^3 \text{ kg m}^{-3}$).

(3 marks)

3.

(a) Briefly describe the four film structure types within the *Thornton Zone model*. Explain with reasons the type most likely to be seen and the effect on the structure of increasing the vapour pressure within the reaction chamber for sputtering deposition, evaporation deposition and the effect if the process was plasma assisted.

(8 marks)

(b) Explain, by use of the *Paschen curve*, what are the major factors effecting production of a stable plasma.

(4 marks)

(c) Compare and contrast the deposition techniques of thermal evaporation and sputtering. Give reasons why sputtering may be preferable to thermal evaporation as a means of depositing thin alloy films on a substrate. Conversely, in which area of film deposition may thermal evaporation be the preferred deposition method?

(5 marks)

(d) A thin film of InAs is to be deposited by *Chemical Vapour Deposition*. An organo-metallic source of trimethyl indium, TMIIn, is used and held at a constant temperature of 35°C . Hydrogen is passed through the TMIIn bubbler at a rate of $20 \text{ cm}^3 \text{ min}^{-1}$. If the reactant ratio (arsine: TMIIn) is 18:1, what flow of arsine gas is required? Assume standard gas volume is 22400 cm^3 , standard pressure 760 mmHg and that the vapour pressure (*VP*) of TMIIn follows the equation below:

$$\log_{10}(VP) = 10.52 - \left(\frac{3014}{T} \right)$$

(3 marks)

4.

(a) Give a brief physical description of the design of a modern *transmission electron microscope* (TEM). Detailed ray diagrams are not required.

(6 marks)

(b) The TEM is most commonly used in either the *bright-field* imaging mode or the *diffraction* mode. Describe the experimental set-up required to operate both these modes (again, detailed ray diagrams are not needed but basic sketches would be informative.)

Discuss *briefly* why these two techniques are so important in the study of materials. Your answer should include the principle and application of diffraction contrast and the method of *selected-area* diffraction.

(7 marks)

(c) A TEM is used to obtain the electron diffraction pattern of a polycrystalline film. The characteristic 'ring pattern' is recorded on a photographic plate. The diameters of the first four rings are measured as 20.0 mm, 28.3 mm, 34.6 mm and 40.0 mm. Given that the specimen has a cubic structure, index the pattern by assigning Miller indices to each ring (reflection). Indicate each step of your reasoning.

(7 marks)

5.

(a) In a bending magnet, electrons follow a circular path. The relativistic emission characteristics result in a 'searchlight' effect for a laboratory observer, with an 'opening angle' which approximates to $1/(2\gamma)$, where γ is the Lorentz factor. Show that by considering Heisenberg's uncertainty principle, the root-mean-square, rms, energy spread can be estimated as

$$\Delta E \geq \frac{2\hbar c \gamma^3}{R},$$

where R is the radius of the electron path and other symbols have their usual meaning. Please indicate each step in your reasoning.

For a given magnetic field B orthogonal to the electron velocity v , a relativistic electron obeys the following equation, where m is the rest mass of the electron,

$$\gamma m \left(\frac{v^2}{R} \right) = evB.$$

Further show that

$$\Delta E \geq \frac{2e\hbar B \gamma^2}{m}$$

(7 marks)

(b) Explain briefly the meaning of *critical photon energy* in the context of bending magnet.

(3 marks)

(c) A more rigorous theoretical treatment leads to an expression for the critical energy as follows,

$$E_c = \frac{3e\hbar B\gamma^2}{2m}$$

Determine the critical energy of a bending magnet operated at 1.27 T in a storage ring with a 1.9 GeV electron beam.

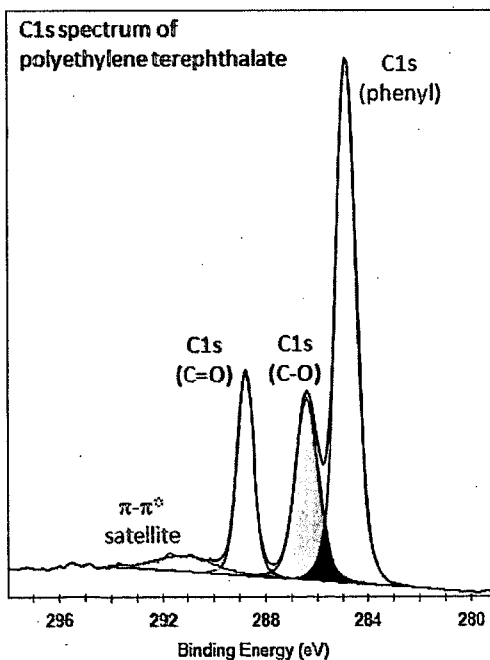
(4 marks)

(d)

(i) Briefly explain the concept of *chemical shift* in the context of photoelectron spectroscopy, using the data from the C1s spectrum of polyethylene terephthalate (shown below) to support your answer.

(ii) The spectrum was taken using Al $K_{\alpha 1}$ X-ray of a photon energy 1486.7 eV. Estimate the kinetic energies associated with the photoelectron peaks.

(iii) The left peak is labelled as $\pi-\pi^*$ satellite. Briefly explain its meaning.



(6 marks)

6.

(a) X-ray diffraction can be performed on a single crystal, or on a powder of small crystallites. Briefly explain one advantage of *single crystal diffraction* and one advantage of *powder diffraction*.

(5 marks)

(b) Briefly explain one advantage of X-ray diffraction and one advantage of neutron diffraction.

(5 marks)

(c) The lattice vectors in the hexagonal close packed lattice are $\mathbf{a} = a\hat{x}$, $\mathbf{b} = \frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}$, $\mathbf{c} = c\hat{z}$. Calculate the reciprocal lattice vector $\mathbf{c}^* = \frac{2\pi(\mathbf{a} \times \mathbf{b})}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}$. You may also use: $\mathbf{c} \cdot \mathbf{c}^* = 2\pi$, $\mathbf{a} \cdot \mathbf{c}^* = \mathbf{b} \cdot \mathbf{c}^* = 0$.

(6 marks)

(d) In an X-ray diffraction experiment, the wavelength of the incident X-rays is $\lambda = 0.4\text{\AA}$ and a first order diffraction peak appears at $\theta = 10^\circ$. According to $\lambda = 2d \sin \theta$ this peak corresponds to a d -spacing of 1.1\AA . If the incident X-ray beam has a spectral line width of $\Delta\lambda = 0.02\text{\AA}$ calculate the width (in terms of θ) of this diffraction peak, assuming that the spectral line width of the incident X-ray beam is the only source of broadening.

(4 marks)

7.

The following is a list of the crystallographic point groups in 2 dimensions:

Point group 1 – Objects only invariant under the identity operator (1).

Point group 2 – Objects only invariant under 2-fold rotation (and 1).

Point group m – Objects only invariant under m (and 1).

Point group 3 – Objects only invariant under for 3+ (and 1).

Point group 4 – Objects only invariant under 4+ (and 2, and 1).

Point group 6 – Objects only invariant under 6+ (and 3+, and 2, and 1).

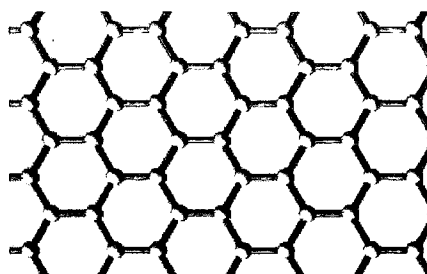
Point group 2mm Objects only invariant under 2, and 2 perpendicular mirror planes (and 1)

Point group 3m Objects only invariant under 3+ and 3 mirror planes at 120°(and 1)

Point group 4mm Objects only invariant under 4+ and 4 mirror planes at 90°(and 2, and 1)

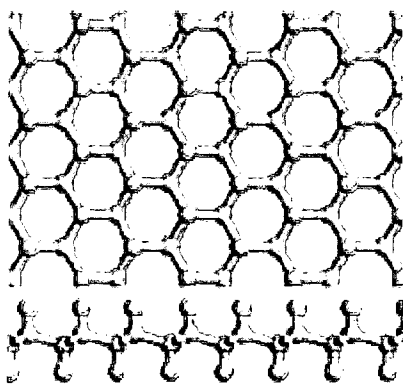
Point group 6mm Objects only invariant under 6+ and 6 mirror planes at 60°(and 2, and 1)

(a) The graphene lattice is shown below. What 2 dimensional crystallographic point group does it belong to?



(4 marks)

(b) The hydrogenated graphene lattice is shown below. What 2 dimensional crystallographic point group does it belong to?



(4 marks)

(c) Phonons in crystalline solids can be detected using inelastic neutron scattering or optical spectroscopy. Optical spectroscopy has the advantages that it can be performed on a much smaller sample, and does not require a neutron source. State one advantage of inelastic neutron scattering?

(4 marks)

(d) The CO_2 molecule, sketched below, is an example of a linear molecule. Sketch the CO_2 molecule in your answer book lying along the x axis. Indicate and write down the 2 axes about which we can excite rotation of the molecule using electromagnetic radiation.



(4 marks)

(e) Heteronuclear diatomic molecules such as CO exhibit vibrational absorption / emission spectra. The energy levels are given by $E_n = (n + \frac{1}{2})\hbar\omega$ where n is an integer and the selection rule for allowed transitions is $\Delta n = \pm 1$. How many optical absorption peaks does a heteronuclear diatomic molecule exhibit?

(4 marks)