

Any calculator, except one with pre-programmable memory, may be used in this examination.

Answer Books A, B and C

LEVEL 2**EXAMINATION CONTRIBUTING TO THE DEGREES OF BACHELOR
OF SCIENCE (BSc) AND MASTER IN SCIENCE (MSci)****PHY2002
Physics of the Solid State****Duration: 3 Hours****Thursday, 10th May 2018 2:30 PM - 5:30 PM**

Examiners: Prof. P. Browning
Dr. P. van der Burgt
and the Internal Examiners

**Answer ALL TEN questions in Section A.
Answer ONE question in Section B.
Answer ONE question in Section C.**

**Use a separate answer book for each Section.
Follow the instructions on the front of the answer book. Enter
your Anonymous Code number and Seat number, but NOT your name.**

THE QUEEN'S UNIVERSITY OF BELFAST
DEPARTMENT OF PHYSICS AND ASTRONOMY

PHYSICAL CONSTANTS

Speed of light in a vacuum	$c = 3.00 \times 10^8 \text{ ms}^{-1}$
Permeability of a vacuum	$\mu_0 = 4\pi \times 10^{-7} \text{ Hm}^{-1}$ $\approx 1.26 \times 10^{-6} \text{ Hm}^{-1}$
Permittivity of a vacuum	$\epsilon_0 = 8.85 \times 10^{-12} \text{ Fm}^{-1}$
Elementary charge	$e = 1.60 \times 10^{-19} \text{ C}$
Electron charge	$= -1.60 \times 10^{-19} \text{ C}$
Planck Constant	$h = 6.63 \times 10^{-34} \text{ Js}$
Reduced Planck Constant	$\hbar = 1.05 \times 10^{-34} \text{ Js}$
Rydberg Constant for hydrogen	$R_\infty = 1.097 \times 10^7 \text{ m}^{-1}$
Unified atomic mass unit	$1u = 1.66 \times 10^{-27} \text{ kg}$ $1u = 931 \text{ MeV}$
1 electron volt (eV)	$= 1.60 \times 10^{-19} \text{ J}$
Mass of electron	$m_e = 9.11 \times 10^{-31} \text{ kg}$
Mass of proton	$m_p = 1.67 \times 10^{-27} \text{ kg}$
Mass of neutron	$m_n = 1.67 \times 10^{-27} \text{ kg}$
Molar gas constant	$R = 8.31 \text{ JK}^{-1} \text{ mol}^{-1}$
Boltzmann constant	$k = 1.38 \times 10^{-23} \text{ JK}^{-1}$
Avogadro constant	$N_A = 6.02 \times 10^{23} \text{ mol}^{-1}$
Gravitational constant	$G = 6.67 \times 10^{-11} \text{ Nm}^2 \text{ kg}^{-2}$
Acceleration of free fall on the Earth's surface	$g = 9.81 \text{ ms}^{-2}$

SECTION A

Use a section A answer book

Answer all 10 questions from this section

1. Demonstrate that five-fold rotational symmetry is not consistent with the conventional definition of a crystalline lattice. **[4]**

2. The Bravais Lattice of zinc blende is Cubic F ($a=b=c$, $\alpha=\beta=\gamma=90^\circ$; face-centred lattice), with the following motif: S at 0,0,0; Zn at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$. Using this information, draw an accurate 2x2 unit cell structure plan of zinc blende viewed down the [001]. **[4]**

3. By plotting all poles related to the general pole in a sketch stereogram, illustrate the operation of the $\bar{6}$ rotoinversion symmetry element. A mirror plane is implied. What is the orientation of this mirror plane with respect to the rotoinversion axis? **[4]**

4. Consider the following Landau-Ginzburg free energy expression:

$$\Delta G = \frac{a}{2}(T - T_c)Q^2 + \frac{b}{4}Q^4$$
 Explain why only even powers in Q appear in this expression and demonstrate explicitly why the Q^2 pre-factor contains a $(T-T_c)$ term. **[4]**

5. By considering the possible relative bond energies associated with bonds that form in a solid solution of two atomic types (A and B for example), demonstrate that ordering and exsolution are often mutually exclusive processes. **[4]**

6. What is the harmonic approximation in the context of developing expressions for phonon dispersion relations and how does this lead to the view of atoms and bonds as balls and springs respectively? **[4]**

7. By sketching frequency-wavevector relations for the monatomic chain and the diatomic chain, discuss and illustrate differences between optic and acoustic phonon modes. **[4]**

SECTION A

8. For electrons, the probability of occupation of a given energy state is determined by the Fermi-Dirac distribution. Sketch the Fermi-Dirac distribution at $T = 0\text{ K}$, label the Fermi energy (E_F) and briefly comment on how its form can be rationalized in terms of Pauli exclusion and thermodynamics. Also sketch the case for an elevated temperature $T_1 > 0\text{ K}$. **[4]**
9. For semiconducting materials, explain how suitable choice of dopant can lead to p- and n-type conduction and include schematic energy band diagrams with Fermi levels at $T = 0\text{ K}$ labelled for each case. Sketch a plot of how the Fermi level is expected to change with temperature for the n-type scenario. **[4]**
10. The electronic structure of sodium is written $1s^2 2s^2 2p^6 3s^1$. Sketch a flat energy band diagram for an isolated sodium atom and for a sodium crystal consisting of N sodium atoms. Label the electron population in each band (i.e. filled band, partially filled, or empty) and comment on how this relates to sodium's expected conductivity behaviour. **[4]**

SECTION B

Use a section B answer book

Answer 1 of the 2 questions in this section

11. The mineral Langisite belongs to the hexagonal crystal system ($a=b \neq c$; $\alpha=\beta=90^\circ$; $\gamma=120^\circ$) with lattice parameters: $a = 3.53\text{\AA}$ and $c = 5.12\text{\AA}$.

- (a) (i) Sketch the relative orientations of the primary axes of the real and reciprocal lattices for Langisite and hence, or otherwise, determine the magnitudes of a^* , c^* and γ^* . **[4]**
- (ii) By plotting an appropriate section of the reciprocal lattice, determine the inter-planar spacing between successive (130) planes in Langisite. **[4]**
- (iii) Extending the analysis in (a)(ii), determine the inter-planar spacing between successive (132) planes in Langisite. **[3]**
- (iv) Hence, or otherwise, determine the angle of intersection between (130) and (132) planes in Langisite. **[3]**
- (b) (i) What is the Ewald Sphere and how can it be used, in conjunction with the reciprocal lattice for a crystal, to determine the orientations in which constructive interference of scattered radiation occurs? **[6]**
- (ii) A single crystal of Langisite is placed in a diffractometer such that $\text{CuK}\alpha$ X-ray radiation (wavelength = 1.54\AA) is incident along the a^* axis. Sketch (to approximate scale) the a^*-c^* section of the reciprocal lattice and the circular trace of the Ewald Sphere associated with this incident X-ray beam. **[5]**

[QUESTION 11 CONTINUED OVERLEAF]

SECTION B**[QUESTION 11 CONTINUED]**

- (iii) The crystal is rotated with respect to the incident X-ray beam about an axis perpendicular to the a^*-c^* reciprocal lattice. At what rotation angle could the 002 reflection in Langisite be observed? **[5]**

[EXAMINATION CONTINUED OVERLEAF]

SECTION B

12. (a) The change in Gibbs Free Energy (ΔG_{mix}), associated with transforming a mechanical mixture of Na and K alkali feldspar into a solid solution, is shown in figure B12.1 below.

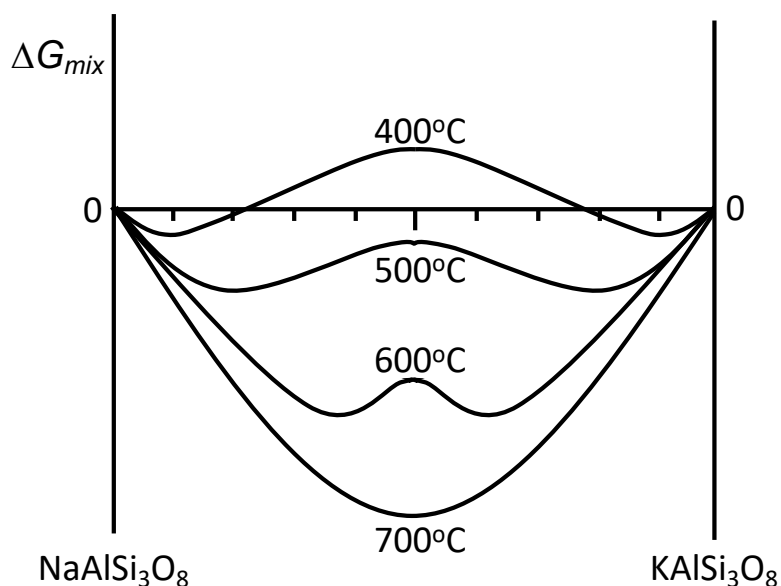


Figure B12.1: Free energy of mixing as a function of composition in the alkali feldspars, at four different temperatures (400°C, 500°C, 600°C and 700°C).

- (i) Describe what is meant by the term “exsolution”? [2]
- (ii) With reference to figure B12.1, comment on the signs of the enthalpy and entropy of mixing in the feldspar system. For a sodium cation, comment on the relative enthalpic energy of another sodium as opposed to a potassium ion being in an adjacent unit cell. [4]
- (iii) For a feldspar of composition $(\text{Na}_{0.5}\text{K}_{0.5})\text{AlSi}_3\text{O}_8$, describe the compositional phases and microstructures that would be expected at 700°C and 400°C. [4]

[QUESTION 12 CONTINUED OVERLEAF]

SECTION B

[QUESTION 12 CONTINUED]

- (iv) Using the information from figure B12.1, construct an accurate composition-temperature phase diagram for the alkali feldspars. [6]

- (b) A typical Landau free energy expression (given in equation B12.1 below) describes the difference in free energy ($G(Q)$) between high symmetry and low symmetry states, as a function of temperature (T), the value of the order parameter (Q), the transition temperature (T_c) and the magnitude of an applied field (H):

$$G(Q) = \frac{a}{2}(T - T_c)Q^2 + \frac{b}{4}Q^4 + \frac{c}{6}Q^6 - HQ \quad \text{equation B12.1}$$

where a , b and c are scalar constants.

- (i) Show that, in the absence of an applied field, the form of the expression given in equation B12.1 predicts the existence of 1st order, 2nd order and tricritical phase transitions. Plot the equilibrium behavior of the order parameter as a function of temperature in each of these cases. [8]
- (ii) When the applied field is non-zero, show that the susceptibility of the order parameter with respect to the field tends to infinity at T_c . By what term is this phenomenon generally known? [6]

SECTION C

Use a section C answer book

Answer 1 of the 2 questions in this section

13. (a) (i) Explain what is meant by the term “heat capacity” and explain how it can be used to experimentally determine the enthalpy (or internal energy) and entropy of a material at a finite temperature. [6]
- (ii) Hence comment on how the separate measurements of the heat capacity of ice and water might allow the prediction of the solid-to-liquid phase transition at 0°C. [4]
- (b) (i) Sketch the form of the heat capacity as a function of temperature, in the absence of any phase transitions, highlighting details at both low and high temperature. Mark out the regions which are well described by the three different models developed by Dulong and Petit (1819), by Einstein (1907) and by Debye (1912). [6]
- (ii) Both Einstein and Debye’s models of heat capacity rely on treating atoms as quantum harmonic oscillators. Assuming each atom exists in a parabolic potential well ($U(x) = \frac{1}{2} kx^2$), show that the eigenfunction $\psi = A \exp\left(-\frac{\alpha x^2}{2}\right)$ is a solution to the one-dimensional time-independent Schrödinger equation: $E\psi = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + U(x)\psi$ and that the ground state ($n=0$) of the atom has an energy of $\hbar\omega/2$. In addition, state the energy of all possible quantum solutions as a function of the quantum number (E_n). [8]
- (iii) Describe the key assumptions used to develop the Einstein model for heat capacity and contrast these assumptions with those made in the Debye model. [6]

SECTION C

14. (a) (i) Describe the physical picture and main assumptions used in the classical Drude theory of metallic conduction. [5]
- (ii) Considering τ as the average time interval for electron collisions, show that, under an applied electric field E , Ohm's law can be derived in the form $J = \sigma E$ where:
- $$\sigma = \frac{ne^2\tau}{m}$$
- and J is current density, σ is the conductivity, and n is number of valence electrons. [8]
- (iii) Given that the conductivity measured in a piece of metal is $\sigma = 5 \times 10^7 \Omega^{-1} \text{m}^{-1}$ at $T = 300 \text{ K}$, estimate the mean free path λ between collisions. Assume the number of valence electrons is $1 \times 10^{29} \text{ m}^{-3}$. [5]
- (iv) The fact that experiments can show up to $\lambda \sim 1 \text{ cm}$ in some high-purity metals at low temperatures is not readily explained by the classical picture. Describe how a quantum picture may account for such observations as temperature is decreased. [2]
- (b) (i) P-n junctions are the key enabling component in semiconductor device technology. Explain, with the aid of an energy band diagram, the equilibrium behaviour at the interface region between p- and n-doped semiconductors, making reference to the terms 'drift current', 'diffusion current' and 'depletion region'. These terms should also be included on your diagram. [7]
- (ii) Sketch the typical current-voltage profile expected for an electrically biased p-n junction. Label the forward and reverse biased regimes as well as the onset of voltage breakdown. [3]

[END OF EXAMINATION]