



**QUEEN'S
UNIVERSITY
BELFAST**

PHY2002

Exam Time Table
Code PHY2002

Answer Books A, B and C.

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

LEVEL 2
Examination contributing to the Degrees of
Bachelor of Science (BSc) and Master in Science (MSci)

PHY2002
Physics of the Solid State

Thursday, 9th May 2019 2:30 PM - 5:30 PM

Examiners: Professor P Browning
Dr P van der Burgt
and the Internal Examiners

Answer ALL TEN questions in Section A for 4 marks each.
Answer ONE question in Section B for 30 marks.
Answer ONE question in Section C for 30 marks.

Use a separate answer book for each Section.
You have THREE hours to complete this paper.

**THE QUEEN'S UNIVERSITY OF BELFAST
SCHOOL OF MATHEMATICS AND PHYSICS**

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 Briefly describe the terms *point group* and *rotoinversion symmetry*. **[4]**

- 2 Draw a diagram representing a primitive and a non-primitive unit cell, and demonstrate that a triangle is not suitable as a unit cell in a crystal lattice. **[4]**

- 3 State the Weiss Zone Law and use it to determine the common direction between (221) and (112) in a triclinic unit cell. **[4]**

- 4 Briefly explain how the strong change in electrical conductivity seen at the Verwey transition in magnetite is related to cationic ordering. At what temperature does the Verwey transition occur. **[4]**

- 5 Phase transitions can be classified as being *first order*, *second order* or *tricritical*. Briefly explain how these classifications are defined and, for each, sketch the form of the order parameter as a function of temperature. **[4]**

- 6 With reference to the interatomic potential, explain what is meant by the “Harmonic Approximation” and hence comment on the validity of considering atomic bonds as Hookean springs. **[4]**

- 7 With reference to phonon dispersion curves, explain how phonon-phonon inelastic interactions can result in Umklapp scattering. **[4]**

- 8 The temperature dependence of electrical resistivity $\rho(T)$ for metals can be expressed via Matthiessen’s rule as a sum of a temperature independent term, a , and a temperature dependent term, $b(T)$:

$$\rho(T) = a + b(T)$$
 What is the fundamental physical mechanism that gives rise to electrical resistance in this picture and why is there no resistance contribution expected from the static crystalline lattice at $T = 0\text{ K}$? What specific mechanisms contribute to a and $b(T)$? **[4]**

- 9 Using illustrations of a populated free-electron parabolic energy-band, explain how a current flow is established when an electric field is applied to a metal. **[4]**

- 10** Explain, with the help of a diagram, the effect of the periodic lattice potential on the energy-wavevector dispersion of a free-electron gas. Label significant points on the wavevector axis in terms of the lattice parameter a . What does the band occupation profile look like for a semiconductor/insulator at $T = 0\text{ K}$? **[4]**

SECTION B

Use a section B answer book

Answer 1 of the 2 questions in this section

- 11 (a) Gallium nitride (GaN), in the form of a wurtzite crystal structure, has a space group $P6_3mc$ (hexagonal crystal system), and lattice parameters $a = 3.21 \text{ \AA}$ and $c = 5.24 \text{ \AA}$.
- (i) Explain what the element 'P' means and what symmetry element does ' 6_3 ' describe [3]
- (ii) Draw a stereogram for the basic hexagonal point group 6, viewed down the c axis. [3]
- (iii) Sketch the relationship between the real and reciprocal lattice axes for GaN, and determine the magnitudes of a^* , c^* and γ^* . [4]
- (iv) With help of the reciprocal lattice, calculate the spacing between the (210) planes in wurtzite GaN. [3]
- (b) (i) Explain what the Ewald sphere is and how can it be used to determine the crystal orientations in an observed diffraction pattern. [4]
- (ii) GaN can also take the form of a zinc blende crystal structure, with a point group $Fm\bar{3}m$ and lattice parameters $a = b = c = 4.27 \text{ \AA}$. A single crystal of GaN $Fm\bar{3}m$ is placed in a diffractometer such that a Cu- $K\alpha$ source ($\lambda = 1.54 \text{ \AA}$) is incident along the a^* axis. Calculate at what angle the 200 reflection will be observed. [3]

[QUESTION 11(b) CONTINUED OVERLEAF]

SECTION B

[QUESTION 11(b) CONTINUED]

- (iii) The Cu- $K\alpha$ source is changed to a Mo- $K\alpha$ source ($\lambda = 0.709 \text{ \AA}$) and the crystal is rotated with respect to the incident X-rays, about an axis perpendicular to the a^* - c^* reciprocal lattice. Draw and use the reciprocal lattice (for GaN $Fm\bar{3}m$) to calculate the angle at which the 002 reflection would be observed. **[6]**
- (iv) Explain why the entire reciprocal lattice is not imaged when a diffraction experiment is carried out on a single crystal. **[4]**

SECTION B

- 12 (a) (i) Consider a solid composed of two different atomic species (A-atoms and B-atoms). The solid has a random distribution of A and B atoms at high temperature but then either undergoes *exsolution* or *ordering* on cooling. Describe what the terms *exsolution* and *ordering* mean and discuss the relative bond energies responsible for each of these processes. In addition, explain why the random solid solution exists at high temperatures. [6]
- (ii) In figure 12.1, the Free Energy of Mixing (ΔG_{mix}) is presented, as a function of composition and temperature, for a solid system composed of A and B atoms. Using the information in the figure, discuss the behaviour of the 50%A - 50%B composition as it cools under equilibrium from 1100°C to 500°C. [4]

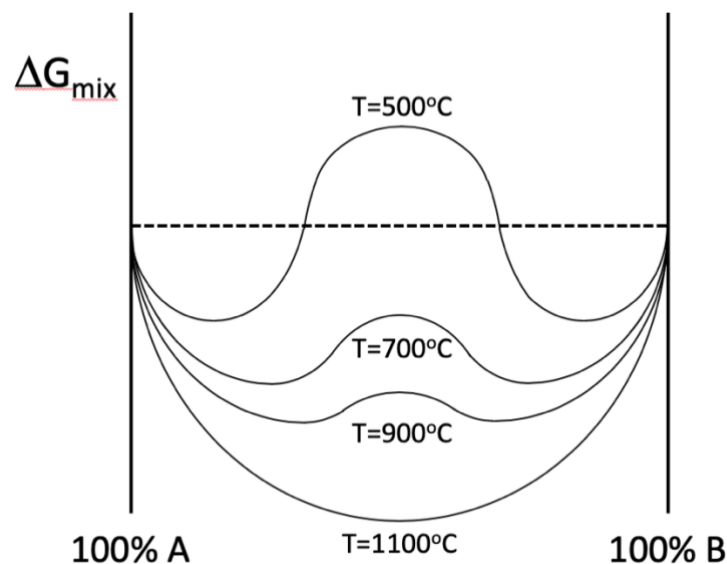


Figure 12.1: Free energy of mixing (ΔG_{mix}) as a function of temperature and composition.

[QUESTION 12 CONTINUED OVERLEAF]

SECTION B

[QUESTION 12 CONTINUED]

- (b) Consider the following Landau Free Energy expression, which gives the change in free energy (ΔG) as a function of the order parameter (Q) under zero applied field:

$$\Delta G = \frac{a}{2}(T - T_c)Q^2 + \frac{b}{4}Q^4 + \frac{c}{6}Q^6 \quad \text{Equation 12.1}$$

- (i) Explain why this expression only contains even powers in Q . **[2]**
- (ii) Considering the Landau expansion up to terms in Q^4 only, rationalise the origin of the $(T - T_c)$ term as part of the prefactor for Q^2 . **[4]**
- (iii) Show that, when the system is in equilibrium, Equation 12.1 can be used to predict first order, second order and tricritical phase transition behaviour. **[6]**
- (iv) Sketch the form of the Landau free energy as a function of the order parameter at temperatures above and below T_c for both first and second order phase transitions. **[4]**
- (v) Under the influence of an externally applied field H , the Landau Free Energy becomes:

$$\Delta G = \frac{a}{2}(T - T_c)Q^2 + \frac{b}{4}Q^4 + \frac{c}{6}Q^6 - HQ \quad \text{Equation 12.2}$$

where Q and H are conjugate variables.

By considering the equilibrium response under applied field, show how transformation plasticity can be inferred from the Landau expression. **[4]**

SECTION C

Use a section C answer book

Answer 1 of the 2 questions in this section

- 13 (a)** By considering the equation of motion for an atom in a 1D monatomic chain (under the harmonic approximation), show that the vibration frequency (ω) can be given as a function of the wavenumber (k) as follows:

$$\omega^2 = \frac{2\mu}{m} \left(\sin \frac{ka}{2} \right)^2 \quad \text{Equation 13.1}$$

where μ is a spring constant, and m the mass, associated with an oscillating atom. **[10]**

- (b)** Einstein developed a model for the heat capacity of solids based on quantum solutions for atoms vibrating within a harmonic potential well, in which the energy difference between vibrational modes (phonons) with successive quantum numbers was $\hbar\omega$.

- (i)** Show that, at a finite temperature T , the average quantum number $\langle n \rangle$ can be given as:

$$\langle n \rangle = \frac{1}{e^{\frac{\hbar\omega}{k_b T}} - 1} \quad \text{Equation 13.2}$$

[8]

- (ii)** Developing Einstein's approach and using the result in (b)(i) above, show that the heat capacity (C) per mole can be given by:

$$C = 3R \left(\frac{\Theta_E}{T} \right)^2 \frac{e^{\frac{\Theta_E}{T}}}{\left(e^{\frac{\Theta_E}{T}} - 1 \right)^2} \quad \text{Equation 13.3}$$

where $\Theta_E = \frac{\hbar\omega}{k_b}$ is the Einstein Temperature, k_b is the Boltzmann constant and R is the molar gas constant. **[8]**

- (iii)** Comment on the validity of the Einstein expression at both high and low temperatures. **[4]**

SECTION C

- 14 (a) (i) Write down a general expression for determining the total number density of occupied electron states n in an energy band in terms of the density of states $D(E)$ and a statistical distribution function $f(E)$ (where E is electron energy). Which specific distribution function is relevant in this case? **[2]**

- (ii) In a semiconductor, the density of states $D(E)$ above the bottom of a conduction band can be modelled by a parabolic function:

$$D(E) = \frac{1}{2\pi^2} \left(\frac{2m_e^*}{\hbar^2} \right)^{\frac{3}{2}} (E - E_c)^{\frac{1}{2}},$$

where E is electron energy, m_e^* is the electron effective mass, and E_c is the conduction band energy minimum.

Show that, for a pure semiconductor, the total carrier density n in the conduction band is given by:

$$n = 2 \left(\frac{m_e^* k_B T}{2\pi \hbar^2} \right)^{\frac{3}{2}} e^{\left(\frac{-(E_c - \mu)}{k_B T} \right)}$$

where μ is the Fermi level (electron chemical potential) and k_b is the Boltzmann constant. In your derivation, you may assume that the energy band-gap is large compared to $k_b T$ and you may also use the standard integral result:

$$\int_0^\infty \sqrt{x} e^{-x} dx = \frac{\sqrt{\pi}}{2} \quad \mathbf{[10]}$$

- (iii) Given that Si and Ge have band-gaps of 1.1 eV and 0.67 eV respectively, and assuming that the effective mass equals the free electron mass in both cases, calculate the carrier densities in their conduction bands at $T = 300 \text{ K}$. [You may assume that the Fermi level (chemical potential) lies in the middle of the band gap.] **[6]**

[QUESTION 14 CONTINUED OVERLEAF]

SECTION C

[QUESTION 14 CONTINUED]

- (b) The following figure shows a calculated electron energy band structure for a crystalline solid:

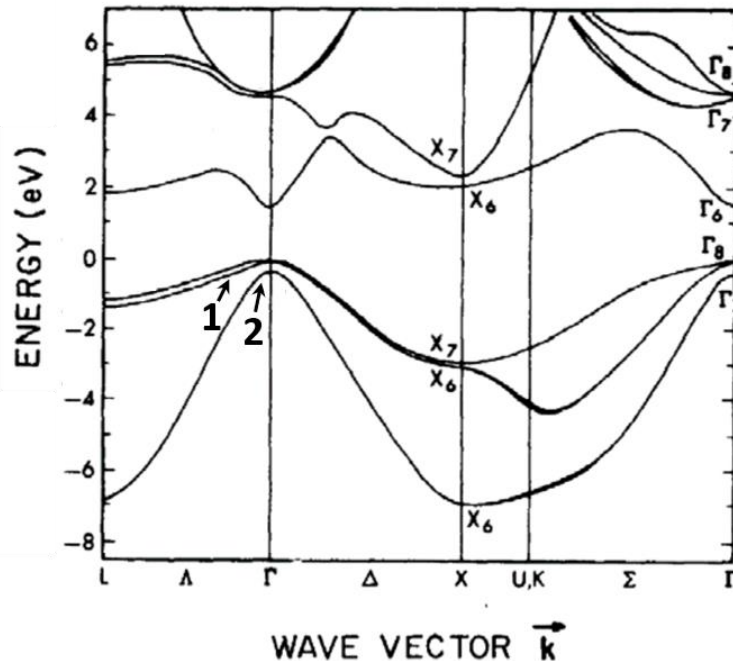


Figure C14.1: A calculated band structure for a crystalline solid. The energy scale is such that the highest occupied states at $T = 0K$ are at zero energy.

- (i) Using the information given in the figure, indicate why this material is unlikely to behave electrically as a metal.
- (ii) Estimate the size of the band gap from the figure and hence deduce whether this material is likely to behave electrically as either a semiconductor or an insulator at room temperature.
- (iii) Would this material be categorised as having a “direct” or “indirect” band gap and why?
- (iv) Consider the energy bands labelled 1 and 2. Justify whether you expect the carrier contributions from each band to be either n- or p-type in character in the vicinity of the Γ point ($k = 0$) at finite temperature. Which of the two bands is expected to have a larger carrier effective mass and why? **[12]**