UNIVERSITY COLLEGE LONDON

University of London

EXAMINATION FOR INTERNAL STUDENTS

For The Following Qualifications:-

B.Sc. *Eng.D.* *M.Sci.*

Physics 3C25: Solid State Physics

COURSE CODE	:	**PHYS3C25**
UNIT VALUE	:	**0.50**
DATE	:	**28-APR-06**
TIME	:	**14.30**
TIME ALLOWED	:	**2 Hours 30 Minutes**

TURN OVER

Answer EVERY question from section A and TWO questions from section B.

The numbers in square brackets in the right-hand margin indicate the provisional allocation of maximum marks per sub-section of a question.

Mass of the electron	m_e	$=$	9.11×10^{-31} kg
Charge on the electron	e	$=$	-1.602×10^{-19} C
Boltzmann's constant	k_B	$=$	1.38×10^{-23} J K^{-1}
Planck's constant/2π	$\hbar$	$=$	1.05×10^{-34} J s

SECTION A

[Part marks]

1. Explain how a real metal can be deformed by stresses that are considerably smaller than its theoretical elastic limit. **[2]**

   Stating your assumptions, estimate the room-temperature concentration of vacancies in a sample of copper, which melts at $1358K$, if the energy difference between a copper atom deep inside the bulk and one attached to the surface is $1.21eV$. **[4]**

2. Sketch the dispersion relation for longitudinal phonons on a linear monatomic chain. In a separate diagram, sketch the dispersion relation for a diatomic chain made up of alternating atoms with two different masses. Be careful to label your axes so that the two relations can be compared. **[3]**

   Explain carefully how the diatomic dispersion relation converts into the monatomic result as the masses of its two atoms are made to be the same. **[3]**

3. According to the tight-binding method, the energy of an electron in a crystal is usually given by a form,

   $$U = -\alpha - \gamma \Sigma_m \exp(-i\mathbf{k} \cdot \rho_\mathrm{m}).$$

   What is the meaning of the symbols α and γ and what range is implied for the sum Σ_m in this expression? **[3]**

   Give an expression for the energy of an electron in a simple cubic lattice with lattice parameter a as a general function of the k-vector according to this model. **[4]**

4. Explain with the aid of a diagram how the k-states of a free electron metal should change under the application of an electric field and show how this explains why the electrical conductivity is proportional to the relaxation time, τ. [3]

   If the effects of impurity scattering and phonon scattering on the electrical conductivity of a metal are described by τ_i and τ_p respectively, and the scattering processes may be assumed to be independent, write down an expression for the resultant scattering time τ when both processes act. [2]

   Describe how you would distinguish between impurity scattering and phonon scattering in measurements of electrical resistance as a function of temperature. [2]

5. Write down an expression for the kinetic energy E_k of a free electron in terms of its wavevector k, and show how the electron mass is related to a derivative of E_k. [3]

   What is meant by the effective mass of a carrier in a semiconductor, and why is it generally different from the mass of a free electron? GaAs has a relatively simple band structure in which electron and hole effective masses are 0.066 and 0.082 times the free electron mass. Why is it that the electrons and holes appear to have similar effective masses? [4]

6. The "law of mass action" for silicon at room temperature is written:

$$np = 2.1 \times 10^{19} cm^{-6}.$$

   Explain the meaning of the symbols and why the numerical value indicates that silicon is a semiconductor. [3]

   If silicon is doped with phosphorus, which has five valence electrons, to a concentration of $3 \times 10^{12} cm^{-3}$, the impurity level lies $0.045eV$ below the conduction band. What will be the electron and hole concentrations at room temperature and where will be the Fermi level? The band gap of silicon is $1.1eV$. [4]

SECTION B

7. (a) State the assumptions that lie behind Bragg's law, $2d\sin\theta = \lambda$, that relates the angle of incidence θ of an X-ray beam of wavelength λ onto planes of a crystal spaced distance d apart which gives rise to a strong diffraction peak . [3]

(b) Draw a detailed diagram showing the positions of the atoms in a crystal of nickel which is known to have the face-centred cubic (fcc) structure with lattice parameter, a_0. Label the axes along the edges of the conventional cubic unit cell and list the coordinates of all the atoms within the cell. Explain how the structure is decomposed into a lattice and a basis, following the cubic convention. [7]

(c) What is the reciprocal lattice of this cubic lattice? Draw a sketch of the reciprocal lattice and label the points according to their Miller indices. Which lattice points correspond to allowed reflections and which are disallowed by the fcc structure? What is the length of the general (hkl) reciprocal lattice vector? Show, with the aid of a sketch, which lattice planes in the crystal correspond to the (111) reciprocal lattice point. [10]

(d) Draw a vector diagram showing how to construct the directions of the incident and exit X-ray beams that correspond to diffraction from the (hkl) reciprocal lattice point. Hence derive an expression for the length of the reciprocal lattice vector and the angle between these two beams, which we will call γ. [5]

(e) In an experiment using X-rays of wavevector $k = 40.8\ nm^{-1}$, a powdered nickel sample is found to produce its first three diffraction peaks at angles, $\gamma = 45.4°, 52.8°$ and $78.0°$. What are the corresponding lengths of the reciprocal lattice vectors? Demonstrate that these are consistent with an fcc structure and deduce the lattice constant a_0. [5]

8. (a) Justify the use of the Lennard-Jones (LJ) potential function to model the interaction potential between two atoms of inert gas separated by a distance, R,

$$U(R) = 4\epsilon\left[\left(\frac{\sigma}{R}\right)^{12} - \left(\frac{\sigma}{R}\right)^{6}\right].$$

What is the meaning assigned to the parameters σ and ϵ? [5]

(b) All the inert gases (except helium) crystallise in the face-centred cubic (fcc) structure. Write down an expression for the cohesive energy of an inert gas solid using the LJ potential. At low temperatures, you can consider this to be purely potential energy. You may use the numerical evaluations of the lattice sums, $P_6 = 14.45392$ and $P_{12} = 12.13188$, which are defined as $P_n = \Sigma_j p_j^{-n}$, where p_j is the distance of the j'th site from the origin of the fcc lattice in units of the nearest-neighbour distance, summed over the entire lattice. [10]

(c) Deduce the equilibrium value of the nearest-neighbour separation, R_0, from your expression. Your answer should be written in terms of the parameters σ and ϵ. [5]

(d) Deduce the *value* of the cohesive energy of neon at low temperature according to this model. The values of σ and ϵ measured for neon gas are $\sigma = 2.74\mathring{A}$ and $\epsilon = 0.0031eV$. [6]

(e) Given that values of σ and ϵ come from gas phase measurements, how good would you expect to be the prediction of the lattice parameter and cohesive energy in the solid? [4]

9. (a) Explain how a contribution to the specific heat of a solid can be obtained by counting all its possible mechanical vibration modes using the assumptions made by Debye. [4]

(b) Derive an expression for the density of modes for the vibration frequencies of a three dimensional monatomic lattice containing N atoms in a total volume V, assuming the speed of sound is v. Hence derive the following expression for the thermal energy of the system in equilibrium at temperature T,

$$U = \int_0^{\omega_D} \left(\frac{V\omega^2}{2\pi^2 v^3}\right) \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} \mathrm{d}\omega.$$

Give an expression for the quantity ω_D and state its meaning. [12]

(c) Now evaluate the low temperature specific heat of the system. State the approximation that is needed to be able to make use of the standard integral [8]

$$\int_0^{\infty} \frac{x^3}{e^x - 1} \mathrm{d}x = \frac{\pi^4}{15}$$

(d) Without detailed calculation, explain what temperature dependence would be expected for the specific heat of a layered material in which the lattice interactions become very weak along one direction in the lattice, *ie* between adjacent layers. [6]

10. (a) What defines the Fermi energy in the free electron model of a simple metal? [4]

(b) Derive an expression for the average kinetic energy of the electrons in a metal in terms of the free electron concentration, N/V, and show that, at low temperatures, this is a simple fraction of the Fermi energy. [10]

(c) Barium is divalent, releasing two metallic electrons per atom, and forms body-centred cubic crystals with cubic lattice parameter 0.503 nm. Calculate the average kinetic energy of these electrons in barium, assuming the free electron model. [6]

(d) What is the reciprocal lattice for barium? Draw a labelled sketch showing the positions of the reciprocal lattice points nearest to the origin and hence the Brillouin zone boundaries in those directions. Does the free electron Fermi surface for barium lie entirely within the first Brillouin zone? What would you expect to happen to the shape of the Fermi surface when the free electron model starts to break down in barium? [10]

END OF PAPER