King's College London

UNIVERSITY OF LONDON

M.Sci. EXAMINATION

CP4477 Electronic properties of solids

Summer 2004

Time allowed: THREE Hours

Candidates must answer THREE questions.
No credit will be given for answering further questions.

The approximate mark for each part of a question is indicated in square brackets.

You must not use your own calculator for this paper.
Where necessary, a College calculator will have been supplied.

TURN OVER WHEN INSTRUCTED

Physical Constants

Permittivity of free space	ϵ_0	=	8.854×10^{-12}	$\mathrm{F\,m^{-1}}$
Permeability of free space	μ_0	=	$4\pi \times 10^{-7}$	$\mathrm{H\,m^{-1}}$
Speed of light in free space	c	=	2.998×10^{8}	$\mathrm{m\,s^{-1}}$
Gravitational constant	G	=	6.673×10^{-11}	$\mathrm{N\,m^2\,kg^{-2}}$
Elementary charge	e	=	1.602×10^{-19}	C
Electron rest mass	m_{e}	=	9.109×10^{-31}	kg
Unified atomic mass unit	m_{u}	=	1.661×10^{-27}	kg
Proton rest mass	m_{p}	=	1.673×10^{-27}	kg
Neutron rest mass	m_{n}	=	1.675×10^{-27}	kg
Planck constant	h	=	6.626×10^{-34}	J s
Boltzmann constant	k_{B}	=	1.381×10^{-23}	$\mathrm{J\,K^{-1}}$
Stefan-Boltzmann constant	σ	=	5.670×10^{-8}	$\mathrm{W\,m^{-2}\,K^{-4}}$
Gas constant	R	=	8.314	$\mathrm{J\,mol^{-1}\,K^{-1}}$
Avogadro constant	N_{A}	=	6.022×10^{23}	$\mathrm{mol^{-1}}$
Molar volume of ideal gas at STP		=	2.241×10^{-2}	$\mathrm{m^3}$
One standard atmosphere	P_0	=	1.013×10^{5}	$\mathrm{N\,m^{-2}}$

a) GaAs has a direct energy gap of 1.43 eV. Its electron, heavy hole and light hole effective masses are respectively 0.072, 0.6 and 0.15 times the free electron mass.

b) A particle of mass m confined in one dimension to a region of width a has energy levels

$$E_n = \frac{h^2}{8ma^2} n^2,$$

where n is an integer.

Answer THREE questions

1) A crystal is represented by a simple cubic lattice with one atom at each lattice site.

a) One lattice site in the simple cubic lattice is chosen to be at the origin of a Cartesian coordinate system. Write down the coordinates of the 6 lattice sites closest to the origin in terms of the bond length a.

[2 marks]

In the tight-binding approximation the energy E of an electron of wavevector $\mathbf{k}$ has the form

$$E = A + B\sum_j \exp\left(-i\mathbf{k}.\mathbf{r}_j\right)$$

when all the atoms are identical and only nearest-neighbours are considered. Here, $\mathbf{r}_j$ is the position of the j^{th} atom relative to the central atom, $A = \langle\phi_1|H|\phi_1\rangle$ and $B = \langle\phi_1|H|\phi_2\rangle$, where ϕ_1 and ϕ_2 are s-like atomic states centred on the atom at the origin and on one of the nearest neighbours respectively, and H is the Hamiltonian.

b) Show that when this theory is applied to the simple cubic lattice, the electronic energy is

$$E = A + 2B\left[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right].$$

[6 marks]

c) Show that surfaces with constant energy are spherical for small $\mathbf{k}$.

[3 marks]

d) The observed spread in energy of the allowed electronic states is 9.0 eV. What is the magnitude of B? State, with justification, whether you expect B to be positive or negative.

[3 marks]

e) If instead the magnitude of B was 1 eV, calculate the effective mass component m_{xx} at the point $k_x = \pi/a$, $k_y = k_z = 0$ for a crystal with $a = 0.37$ nm.

[3 marks]

f) The values of k_x, k_y and k_z are equi-spaced with separations $2\pi/L$, where L is the edge-length of the crystal. Derive an expression for the density $g(E)$ of electron states in the limit of small $\mathbf{k}$ in terms of A, B and L. Sketch $g(E)$ as a function of E in this limit.

[3 marks]

2)

a) Outline how one could make a 'quantum wire' of GaAs embedded inside a crystal of AlGaAs. Include a description of the equipment required.

[5 marks]

b) In the longitudinal (z) direction in the wire, the energy of an electron is assumed to depend on the wavenumber k as $E = \hbar^2 k^2/2m^*$, and the wavefunctions of the electron are of the form $\psi(z) = \exp(ikz)/\sqrt{L}$, where L is the length of the wire. Use cyclic boundary conditions to show that the separation of the allowed values of k is $\Delta k = 2\pi/L$. Hence show that the density of electron states as a result of motion in the z direction is of the form

$$g(E) = \frac{2L}{h}\sqrt{\frac{m^*}{2E}}.$$

[4 marks]

c) Sketch a plot of the density of electron states against the total energy of the electrons, allowing for the 'motion' in the x and y directions.

[2 marks]

d) A quantum wire has a square cross-section of width $a = 8.0$ nm. It is excited to create a low density of holes and electrons trapped in the wire. Adapting the information given at the head of the examination paper, estimate the lowest energy, in eV, of the luminescence that is emitted when an electron and a hole recombine.

[4 marks]

e) Luminescence observed along the x axis (which is perpendicular to the length of the quantum wire) is detected with its electric vector polarised parallel to the y axis. Show that the luminescence occurs only for transitions involving an electron and a hole with identical quantum numbers n_x.

[5 marks]

3)

a) A metal has a free-electron density of $\rho = 6.0 \times 10^{28}$ m^{-3}. Show that, in the free-electron model, the magnitude of the wavevector at the Fermi surface of the metal is $k_\mathrm{F} = 1.21 \times 10^{10}$ m^{-1}.

You may assume that in the free-electron theory, the density of electron states at energy E is

$$g(E) = C\sqrt{E},$$

where

$$C = \frac{8\sqrt{2}\pi m_e^{\frac{3}{2}} V}{h^3},$$

and V is the volume of the metal.

[4 marks]

b) The metal is placed at a very low temperature in a magnetic field of 0.5 Tesla. The cyclotron energy of an electron as a result of its motion in the field is of the form $\left(n + \frac{1}{2}\right) \hbar\omega_c$ where n is an integer. By equating the kinetic energy of a free electron to its cyclotron energy in a magnetic field, or by any other method, calculate the highest value of n for an occupied state.

[3 marks]

c) The coupling of the spin of the electron to a magnetic field changes its energy by $m_s g_s \mu_B B$ where $m_s = \pm\frac{1}{2}$, $g_s = 2$, and $\mu_B = e\hbar/m_e$ is the Bohr magneton. Write down an expression for the difference ΔE_s in energies of the 'spin-up' and 'spin-down' states for an electron in a magnetic field of strength B. What is the ratio of ΔE_s and $\hbar\omega_c$ if the effective mass of the electron in the metal is $0.1\ m_\mathrm{e}$?

[3 marks]

d) Show that the period of de Haas van Alphen oscillations is $\Delta(1/B) = (2\pi)^2 e/hS$ where S is the area in k-space that is enclosed by the orbit.

[4 marks]

e) Calculate the period of the de Haas van Alphen oscillations in the metal using the value of k_F from part (a).

[3 marks]

f) In practice a de Haas van Alphen oscillation with a significantly longer period is detected when the magnetic field is applied to the metal along certain crystallographic directions. Explain why this longer period may be observed.

[3 marks]

4)

a) The electrons in a two-dimensional system are represented by free-electron states. For a two-dimensional crystal of edge L, the allowed values of the wavenumbers are separated by $\Delta k = 2\pi/L$. Show that the density $g(E)$ of electron states at energy E is given by

$$g(E) = \frac{4\pi m^* L^2}{h^2},$$

where m^* is the effective mass of the electrons.

[3 marks]

b) A layer of GaAs of thickness 3.0 nm is embedded in AlGaAs. Using the data and information at the head of the paper, estimate the energies in eV of the first ($n = 1$) and second ($n = 2$) quantised energy levels.

[3 marks]

c) The structure is doped with donors so that there are 10^{16} m^{-2} free electrons in the layer. Show that the electrons only occupy the $n = 1$ quantum state of the layer. Calculate, in eV, the highest energy of the electrons relative to the bottom of the conduction band in the GaAs layer.

[4 marks]

d) A magnetic field of strength $B = 10.34$ Tesla is applied perpendicular to the layer, producing Landau levels with spin-up and spin-down. Calculate the number of electron states in each of these levels. How many Landau levels are completely filled at this magnetic field?

[4 marks]

e) The transverse resistance ρ_T is defined as $\rho_T = E/J$ where E is the electric field created by the Hall effect and J is the current flowing divided by the width of the layer. When the magnetic field is increased slightly, ρ_T is found to be constant. Calculate the value of ρ_T, and show how you may check your answer from the known values of h and e.

[6 marks]

5)

a) A spin-only paramagnetic system has n non-interacting magnetic moments per unit volume, each with total angular momentum $J = 1$ and Landé factor $g = 2$. Show that the magnetisation per unit volume in a magnetic induction field B, at temperature T, may be written as

$$M(y) = \frac{4n\mu_B \sinh(y)}{1 + 2\cosh(y)}$$

where $y = 2\mu_B B / k_B T$ and μ_B is the Bohr magneton.

[5 marks]

b) Show that at low enough values of B, or high enough temperatures, the magnetic susceptibility of this system may be written as

$$\chi = \frac{C}{T}$$

and obtain an expression for C.

[4 marks]

c) Sketch $M(y)$ as a function of y and give its saturation value for large y.

[1 mark]

d) If the magnetic moments now interact, the effective field acting on each ion may be written as $B = B_0 + \lambda M$, where B_0 is the external applied field, M is the magnetisation per unit volume, and λ is a molecular field constant. Show that the metal becomes ferromagnetic in zero applied field below a temperature

$$T = \frac{8n\lambda\mu_B^2}{3k}.$$

[5 marks]

e) For small y, the magnetisation $M(y)$ may be written as $M(y) = ay - by^3$ where a and b are positive. Using the molecular field model for ferromagnetism, show that at $T = T_C$ the magnetisation $M(B, T_C)$ is proportional, for small fields, to $B^{1/3}$.

[5 marks]