King's College London

UNIVERSITY OF LONDON

M.Sci. EXAMINATION

CP/4477 Electronic properties of solids

Summer 2001

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

Avogadro number $N_A = 6.022 \times 10^{23}$ mole^{-1}

Boltzmann constant $k = 1.381 \times 10^{-23}$ J K^{-1}

Planck constant $h = 6.626 \times 10^{-34}$ J s

Charge of a proton $e = 1.602 \times 10^{-19}$ C

Rest mass of an electron $m_0 = 9.109 \times 10^{-31}$ kg

Bohr magneton $\mu_B = 9.274 \times 10^{-24}$ J T^{-1}

Permeability of free space $\mu_0 = 4\pi \times 10^{-7}$ H m^{-1}

Permittivity of free space $\epsilon_0 = 8.854 \times 10^{-12}$ F m^{-1}

Answer THREE questions

1) In free-electron theory, the density of electron states at energy E is $g(E) = c\sqrt{E}$, where $c = 8\sqrt{2}\pi m_o^{3/2} V/h^3$, and V is the volume occupied by the electrons.

Derive an expression for the Fermi energy E_F at 0 K and show that the total energy of a gas containing N electrons at 0 K is $E_t = (3/5)NE_F$.

[3 marks]

The bulk modulus B of a crystal is defined as the change in pressure P required to produce a fractional change in volume V:

$$B = -V\left(\frac{\mathrm{d}P}{\mathrm{d}V}\right)_T,$$

and P can be related to E_t by $PdV = -dE_t$. Calculate the value of B at 0 K predicted by free-electron theory for metallic potassium given that its density is 862 kg m^{-3} and its atomic weight is 39.1. (The experimental value measured at room temperature is 3.0 GPa).

[10 marks]

Sketch the distribution of filled electron states, as a function of energy, for the electron gas at 0 K and at $T > 0$ K, and write down an approximate expression for the increase in electron energy as a function of T.

[2 marks]

Estimate the change in B as the temperature increases from 0 K to 300 K, assuming that the volume of the crystal is essentially constant over this temperature range.

[5 marks]

2) The electrons in a two-dimensional system are represented by free electron states. Derive an expression for the density of electron states and thereby show that it is independent of the energy of the electrons.

[3 marks]

A quantum layer 1 mm square is embedded in a semiconductor and is doped with donors so that there are 10^{12} cm^{-2} electrons in the layer. The layer is sufficiently thin that only the lowest quantised energy level need be considered. A magnetic field of 5 Tesla is directed perpendicular to the quantum layer. How many Landau levels are completely filled with electrons?

[4 marks]

The field is increased so that precisely 8 Landau levels are filled. What is the strength of this field B_8? What is the energy of the maximum filled Landau level, if the quantum layer is made of GaAs?

[3 marks]

The transverse resistivity 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 (1 mm) of the layer. Calculate the value of ρ_T for the quantum layer at the field B_8.

[6 marks]

Comment on the importance of measuring ρ_T, and show how you may check your calculated value from the known values of h and e.

[4 marks]

3) In a crystal of silicon, an interstitial oxygen atom is stable at approximately the midpoint of one of the identical Si–Si bonds. By minimising the free energy ($F = U - TS$), show that, in thermal equilibrium, there are $n \approx N \exp(-E_0/kT)$ interstitial oxygen atoms in the crystal, where N is the number of interstitial sites and E_0 is the energy required to introduce one oxygen atom from the surface, assuming that $n << N$.

[You may assume Stirling's formula, that $\ln p! \approx p \ln p - p$].

[6 marks]

The diffusion coefficient D of an impurity atom is defined in terms of the number j of atoms crossing unit area in unit time and the gradient $\mathrm{d}n/\mathrm{d}x$ of concentration by $j = -D\mathrm{d}n/\mathrm{d}x$. Representing the silicon lattice by a simple cubic lattice, show that

$$D = \tfrac{2}{3}\nu a^2 \exp\left(-E_b/kT\right)$$

where a is the distance between equivalent sites for the oxygen atoms, ν is the vibrational frequency of the oxygen atom, and E_b is the energy barrier to diffusion.

[5 marks]

Evaluate the mean distance between the oxygen atoms in a crystal of silicon that is grown at 1680 K in an oxygen-rich environment, given that the best fit to the solubility data is obtained with $E_0 = 1.52$ eV and $N = 9.0 \times 10^{22}$ cm^{-3}.

[2 marks]

Estimate the time taken for two oxygen atoms to come into neighbouring sites in the crystal when it is heated to 720 K, given that the experimental data for diffusion are best fitted using $D = D_0 \exp(-E_b/kT)$ with $E_b = 2.5$ eV and $D_0 = 0.13$ cm^{2}s^{-1}.

[2 marks]

Describe qualitatively the behaviour of the oxygen atoms in a crystal of silicon that is grown at 1680 K in an oxygen-rich environment, suddenly cooled to room temperature, and subsequently heated slowly to 720 K ($\approx 450°$C).

[3 marks]

Outline an experimental technique by which the diffusion could be monitored.

[2 marks]

4) Answer all parts.

a) The area of $\mathbf{k}$-space enclosed by the orbit of a nearly-free electron is πk^2 and the wavevector is related to the electron's energy E by $k = \sqrt{2mE}/\hbar$. What is the value of the area for electrons in metallic copper for which the de Haas van Alphen oscillations occur at equal intervals of reciprocal field of $\Delta(1/B) = 8.2 \times 10^{-6}\ \mathrm{T}^{-1}$? Why are significantly different values of $\Delta(1/B)$ also detected for electrons at the Fermi surfaces of copper?

[6 marks]

b) The tight-binding approximation applied to a simple cubic lattice in which only nearest neighbours interact gives electronic energy levels of

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

where a is the nearest neighbour separation, A and B are the one- and two- atom interaction terms, and the k_i are the components of the electron wavevector. It is found that a certain material can be modelled approximately by using $A = -4$ eV, $B = -2$ eV and $a = 0.2$ nm.

Calculate the value of the effective mass of the electrons as $\mathbf{k} \to 0$ and show that it is isotropic (has the same value for all directions).

[4 marks]

Show that for all $\mathbf{k}$, all off-diagonal masses m_{ij}, with $i \neq j$, are infinite. Comment on the physical meaning of this result.

[2 marks]

c) By considering the displacement of an electron cloud from its equilibrium position, estimate the energy quantum of the bulk plasmon for a semiconductor with an electron density of $2.0 \times 10^{29}\ \mathrm{m}^{-3}$, relative permittivity of 11.6, and an electron mass equal to $0.5m_0$.

Comment on the influence of collective electron motions on the value of the Fermi energy in a semiconductor.

[4 marks]

d) The ionisation energy of a hydrogen atom is 13.6 eV, and the Bohr radius scales in proportion to the permittivity of the environment and inversely with the mass of the system. Estimate the ionisation energy of an exciton in silicon for which the relative permittivity is 11.6 and the effective masses of the electrons and holes are, respectively, $0.6m_0$ and $0.16m_0$.

Comment on the importance of electron-hole interactions in calculations of the electron band structure in semiconductors.

[4 marks]

5(a) A hypothetical metal has n non-interacting localised moments per unit volume, each with allowed magnetic quantum numbers $m_J = \pm\frac{1}{2}$, spin g-factor $g = 2$, and hence magnetic moments $\mu = m_J g \mu_B = \pm\mu_B$. Show that the magnetic susceptibility (Curie susceptibility) of the localised moments in a magnetic induction field B and at temperature T is given by :

$$\chi = \frac{n\mu_0\mu_B}{B}\tanh\left(\frac{\mu_B B}{kT}\right).$$

[4 marks]

Derive the limiting value for the susceptibility in low fields.

[2 marks]

(b) Show that the magnetic susceptibility of the conduction electrons of the metal (the Pauli susceptibility) is given by

$$\chi_P = n\mu_0\mu_B^2 D(E_F)$$

where $D(E_F)$ is the density of conduction band states at the Fermi energy.

[6 marks]

(c) Consider a heavy Fermion metallic compound which has an atomic weight (per formula unit) of 800, a density of 20 g cm^{-3}, and an exceptionally high density of states at the Fermi energy of $D(E_F) = 1.1 \times 10^{21}$ (formula unit)$^{-1}$ J^{-1}.

(i) Calculate the Pauli susceptibility of this metallic system.

[4 marks]

(ii) Calculate the ratio of its Pauli susceptibility to its Curie susceptibility at a temperature of 10 K. Assume, as in part (a) of this question, that it has localised moments with allowed magnetic quantum numbers $m_J = \pm\frac{1}{2}$, and spin g-factor $g = 2$.

[4 marks]