King's College London

UNIVERSITY OF LONDON

M.Sci. EXAMINATION

CP/4477 Electronic properties of solids

Summer 2000

Time allowed: TWO 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

Boltzmann constant $k = 1.38 \times 10^{-23}$ JK^{-1}

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

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

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

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

Permeability of free space $\mu_o = 4\pi \times 10^{-7}$ Hm^{-1}

Permittivity of free space $\epsilon_o = 8.854 \times 10^{-12}$ Fm^{-1}

GaAs has a direct energy gap of 1.43 eV, a relative permittivity of $\epsilon = 10.9$, and a lattice constant of 0.565 nm. Its electron, heavy hole and light hole effective masses are 0.072, 0.6 and 0.15 times the free electron mass.

Answer THREE questions

1) One lattice site in a body-centred cubic lattice is chosen to be at the origin of a Cartesian coordinate system. Write down the coordinates of the 8 lattice sites closest to the origin.

[4 marks]

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

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

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 non-degenerate states on the atom at the origin and on one of the nearest neighbours respectively, and H is the Hamiltonian.

Show that when this theory is applied to a body-centred cubic crystal with one atom at each lattice site, the electronic energy is

$$E = A + 8B\cos(k_x a/2)\cos(k_y a/2)\cos(k_z a/2)$$

where a is the length of the edge of the unit cube.

[8 marks]

Show that surfaces with constant energy are spherical when $\mathbf{k} \to 0$.

[4 marks]

Find the effective mass component m_{zz} in terms of B at the point $k_x = k_y = 0$, $k_z = \pi/a$.

[4 marks]

2) Sodium (Na) crystallises in the body-centred cubic lattice with lattice vectors $\mathbf{a}_1 = (a/2)(\bar{1}, 1, 1)$, $\mathbf{a}_2 = (a/2)(1, \bar{1}, 1)$, $\mathbf{a}_3 = (a/2)(1, 1, \bar{1})$ where a is the length of the unit cube. The volume of the unit cell is $V = a^3/2$. Given that the reciprocal lattice vectors are $\mathbf{b}_i = (2\pi/V)\mathbf{a}_j \times \mathbf{a}_k$, show that the smallest separation of points in the reciprocal lattice is $2^{3/2}\pi/a$.

[4 marks]

State the assumptions of the free electron theory of metals.

[4 marks]

Using the free-electron approximation, write down the time-independent Schrödinger equation for an electron in a cubic crystal of edge length L. Show that

i) the allowed wavevectors have components $k_i = 2\pi n_i/L$, where n_i is an integer, and

ii) at 0 K the Fermi surface occurs at $k_F = 3.9/a$.

[8 marks]

Confirm that the Fermi surface lies entirely within the first Brillouin zone, and comment on the relevance of this result to the validity of applying the free-electron model to sodium.

[4 marks]

3) GaAs is a direct-gap semiconductor with an energy gap of $E_g = 1.43$ eV.

State the energy and wavevector selection rules for absorption of light of wavelengths near 860 nm. By comparing the wavevector of light of these wavelengths with the size of the Brillouin zone, simplify the wavevector selection rule.

[3 marks]

Assuming that the energy of an electron at an energy E above the bottom of the conduction band is proportional to the square of the electron's wavevector, derive an expression for the density of electron states in the conduction band.

[5 marks]

By considering the effective masses for electrons and holes given in the information at the head of the paper, deduce a power law for the dependence of the absorption coefficient on the photon energy in a valence-band to conduction-band transition.

[4 marks]

A donor is introduced into the GaAs. Assuming that simple effective-mass theory is valid, estimate the spread in wavevector space of the ground state of the donor. You may assume that the Bohr radius of the H atom in its ground state is given by $r = \left(4\pi\epsilon_o\hbar^2\right) / \left(me^2\right)$.

[4 marks]

Give one reason why you expect the simple effective mass theory to be approximate, and discuss qualitatively the effect of allowing for this approximation.

[2 marks]

Estimate the concentration of donors at which interactions will take place between the ground states of the donors.

[2 marks]

4) *Data for GaAs are given at the head of the paper.*

Estimate the binding energy (in eV) of an exciton in bulk GaAs. You may assume that the ionisation energy of a hydrogen atom is

$$\frac{me^4}{8(\epsilon_o h)^2} = 13.6 \quad \text{eV}.$$

[3 marks]

A quantum well, 5 nm thick, of GaAs is sandwiched between thick layers of an AlGaAs alloy which is lattice-matched to GaAs. Assuming that a particle of mass m in an infinitely deep potential well of width a has energy levels

$$E = \frac{h^2}{8ma^2} n^2, \quad n = 1, 2 \ldots,$$

calculate the lowest energy photon that can be absorbed in the well. (The AlGaAs alloy can be taken to have a band gap of 2 eV, and the valence band offset with GaAs is 0.34 eV.)

[6 marks]

Explain why, when light travels perpendicularly through the well, the creation of a hole in its $n = 1$ state and an electron in its $n = 2$ state has a negligible probability for all wavelengths of light.

[4 marks]

Given that the density of electron states for an electron that is constrained to move in two dimensions is $m/(\pi\hbar^2)$ per unit area, sketch the shape of the absorption spectrum for transitions in the well, including the excitonic transitions.

[3 marks]

A magnetic field B is applied perpendicular to a quantum layer of GaAs. Show that for a sufficiently small number of free electrons in the layer there are $N = eB/\hbar$ states in each occupied Landau level.

[4 marks]

5 (a) Consider a paramagnetic system with n non-interacting magnetic moments per unit volume, each with total angular momentum J, magnetic quantum number m_J, and Landé factor g. Show that the average magnetic moment in a magnetic induction field B, at temperature T, may be written as :

$$\langle \mu \rangle = \frac{\sum_{m_J} g\mu_B m_J \exp(g\mu_B m_J B/kT)}{\sum_{m_J} \exp(g\mu_B m_J B/kT)}.$$

[4 marks]

This expression may also be written as

$$\langle \mu \rangle = g\mu_B J \; F(J, y)$$

where the Brillouin function $F(J, y)$ is

$$F(J, y) = \frac{2J+1}{2J} \coth\left(\frac{2J+1}{2J} y\right) - \frac{1}{2J} \coth\left(\frac{y}{2J}\right)$$

and $y = (g\mu_B JB)/(kT)$.

By considering the behaviour of $F(J, y)$ at small values of y, show that the magnetic susceptibility χ of this system may be written as :

$$\chi = C/T$$

where $C = [n\mu_o \mu_B^2 g^2 J(J+1)]/3k$.

[10 marks]

(b) The rare earth element praesodymium (Pr) has two 4f electrons in an unfilled shell. Use Hund's rules to deduce J, and hence the magnetic moment of an isolated Pr ion.

[3 marks]

You may assume that the Landé g-factor is given by:

$$g = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}.$$

(c) Calculate the paramagnetic susceptibility of a system containing Pr ions with a density of 10^{28} m^{-3} at a temperature of 300 K.

[3 marks]