King's College London

UNIVERSITY OF LONDON

B.Sc. EXAMINATION

CP/3402 Solid State Physics

Summer 1998

Time allowed: THREE Hours

Candidates must answer SIX parts of SECTION A, and TWO questions from SECTION B.

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

Separate answer books must be used for each Section of the paper.

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

TURN OVER WHEN INSTRUCTED

<u>Fundamental constants</u>

Reduced Planck constant	$\hbar$	=	1.055×10^{-34} J s
Elementary charge	e	=	1.602×10^{-19} C
Rest mass of an electron	m_e	=	9.109×10^{-31} kg
Energy equivalence	1 J	=	6.242×10^{18} eV
Boltzmann constant	k_B		(value not needed)
Avogadro number	N_A		(value not needed)

SECTION A - answer six parts of this section

1.1) Describe the diamond crystal structure.

Assuming that the atoms behave as hard spheres in close contact, show that the packing fraction is $\sqrt{3}\,\pi/16$.

[7 marks]

1.2) Sketch the ω vs. k dispersion curves for the vibrational frequencies of a linear chain of atoms with two different masses placed alternately. (ω is the angular frequency and k is the wavenumber.)

Explain why the *optical branch* and the *acoustic branch* are so named.

[7 marks]

1.3) Sketch the variation of specific heat capacity for a non-metallic crystal as a function of temperature, as predicted by the Debye equation. Describe, without derivation, how the heat capacity C_v varies with temperature T near T = 0 K, for (a) a non-metallic crystal and (b) a metallic crystal.

[7 marks]

1.4) State Mattheisen's rule relating to the variation of the resistivity of metals with temperature. By expressing the resistivity ρ as $m_e/(ne^2\tau)$, where n is the concentration of conduction electrons and τ is the relaxation time, show how this rule originates.

[7 marks]

1.5) Write down the expression for the effective mass of holes in the valence band of a semiconductor.

Silicon has two valence bands, degenerate at $k = 0$, with masses $m_{h1} = 0.49\ m_e$ and $m_{h2} = 0.16\ m_e$, and a third band of mass $m_{h3} = 0.25\ m_e$ split off by 35 meV. Sketch the E vs. k curves to illustrate this valence band structure, carefully identifying each of the bands.

[7 marks]

1.6) Explain how elements from group V of the periodic table form substitutional donors in silicon. Estimate the ionisation energy of such a donor using the hydrogen model analogy, given that the ionisation energy of the hydrogen atom is

$$E_1 = -\frac{m_e e^4}{2\hbar^2 (4\pi\varepsilon_0)^2} = -13.6\ \text{eV}$$

where ε_0 is the permittivity of free space.

Note: For Si the effective mass of the electrons is $m_e^* = 0.33\ m_e$, and the relative permittivity is $\varepsilon_r = 11.7$.

[7 marks]

1.7) Explain what is meant by a *depletion layer* in a p-n junction. Describe how the formation of this layer accompanies the build-up of a potential barrier V_0.

Explain, briefly, why the p-n junction acts as a rectifier.

[7 marks]

1.8) Explain what is meant by the critical field B_c and the critical temperature T_c for a type I superconductor. Sketch the relationship between B_c and T_c for a typical type I superconductor.

Explain, briefly, the Silsbee hypothesis.

[7 marks]

SECTION B - answer two questions

2.) Explain the meanings of the terms in the expression for the structure factor in relation to scattering of X-rays from a crystalline solid:

$$F_{\mathrm{hkl}} = \sum_j f_j \exp\{2\pi i\,(h\,x_j + k\,y_j + l\,z_j)\}.$$

[4 marks]

Hence show that crystals, with the face-centred cubic structure, scatter X-rays only if *h*, *k* and *l* are all odd or all even.

[8 marks]

Describe how the X-ray diffraction pattern of a powdered crystalline solid may be obtained using a Debye-Scherrer camera. Explain how the pattern may be used to obtain information about the crystal structure.

[8 marks]

The sample in a Debye-Scherrer camera of radius 57.3 mm is finely powdered copper and is irradiated with X-rays (from a synchrotron) with wavelength 0.21 nm. Show that 4 ‘rings’ will be observed on the film, and calculate the diameters of the largest and smallest rings. (Copper has the face-centred cubic structure with a lattice constant of 0.361 nm.)

[10 marks]

3.) State the assumptions made by Einstein to obtain an expression for the temperature-dependence of the heat capacity of a crystalline solid.

[3 marks]

Show that, at temperature T, the average energy of a quantum oscillator with angular frequency ω is

$$\overline{E} = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{\left[\exp(\hbar\omega / k_B T) - 1\right]}$$

[12 marks]

Hence show that the Einstein expression for the heat capacity per mole may be written as

$$C = 3N_A k_B \left(\frac{\theta_E}{T}\right)^2 \frac{\exp(\theta_E / T)}{\left[\exp(\theta_E / T) - 1\right]^2}$$

[5 marks]

where θ_E is the Einstein temperature, ω_E is the Einstein frequency and $\theta_E = \hbar\omega_E/k_B$. Discuss the behaviour of this expression at (a) high temperature and (b) low temperature.

[6 marks]

The Einstein temperature of diamond is 1320 K. Show that at room temperature (293 K) the heat capacity is less than a quarter of the high-temperature limit.

[4 marks]

4.) Krönig and Penney showed that electrons in a one-dimensional crystal, moving in a periodic potential with the same periodicity as the lattice, can have energies E related to the wavenumber k by

$$\cos(ka) = \cos(\lambda a) + \alpha \sin(\lambda a),$$

where $\alpha = m_e \boldsymbol{V}/\lambda\hbar^2$, $\lambda = (2m_e E)^{1/2}/\hbar$, a is the period of the lattice, and $\boldsymbol{V}$ represents the strength of the potential barrier between the unit cells.

Using a diagram, show how this relationship leads to a situation in which allowed energy bands are separated by forbidden energy bands. Show further that when $\boldsymbol{V} = 0$ (as in a metal) the solution reduces to the free-electron parabola $E = \hbar^2 k^2/2m_e$.

[15 marks]

For a one-dimensional crystal with atoms separated by 3×10^{-10} m, and a potential barrier of strength $\boldsymbol{V} = 2 \times 10^{-9}$ eV m, show that:

(a) electrons of energy 15 eV will lie in an allowed band;

(b) electrons cannot have an energy of 20 eV because this energy will lie in a forbidden region.

[15 marks]

5.) For a semiconductor at temperature T, show that the concentrations of electrons in the conduction band and holes in the valence band are respectively

$$n = N_C \exp\left[\frac{-(E_g - E_F)}{k_B T}\right]$$
$$p = N_V \exp\left[\frac{-E_F}{k_B T}\right]$$

where E_g and E_F are the energy gap and Fermi energy, respectively. Explain the meanings of the parameters N_C and N_V.

[20 marks]

At temperatures above 270 K, the energy gap for silicon is given approximately by $E_g = E_0 - \alpha T$, where E_0 and α are constants. Show that, for intrinsic silicon, a plot of [ln(n_i) – 1.5 ln(T)] versus $1/T$ has a gradient of $-E_0/2k_B$. (n_i is the intrinsic electron concentration.)

[10 marks]

You may assume that, for a three-dimensional semiconductor of volume V, the density-of-states functions for electrons in the conduction band and holes in the valence band are, respectively,

$$g_C(E) = \left[\frac{V}{2\pi^2\hbar^3}\right]\left(2m_e^*\right)^{3/2}\left(E - E_g\right)^{1/2}$$

$$g_V(E) = \left[\frac{V}{2\pi^2\hbar^3}\right]\left(2m_h^*\right)^{3/2}\left(-E\right)^{1/2}$$

where the symbols have their usual meaning.

Assume also that, provided the Fermi Level is at least a few $k_B T$ away from the band edges, the probability that an electron energy level is occupied at temperature T is approximately given by

$$f(E) \approx \exp[-(E - E_F)/k_B T].$$

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