King’s College London

UNIVERSITY OF LONDON

B.Sc. EXAMINATION

CP/3402 Solid state physics

Summer 2000

Time allowed: THREE Hours

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

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

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

<u>Fundamental constants</u>

Planck constant	h	=	6.626×10^{-34} J s
Elementary charge	e	=	1.602×10^{-19} C
Rest mass of an electron	m_e	=	9.109×10^{-31} kg
Permittivity of free space	ε_0	=	8.854×10^{-12} F m^{-1}
Boltzmann constant	k_B	=	1.381×10^{-23} J K^{-1} = 8.617×10^{-5} eV K^{-1}
Avogadro number	N_A	=	6.022×10^{23} mol^{-1}

SECTION A – Answer SIX parts of this section

1.1) Describe the CsCl crystal structure.

The ionic radii of Cs^+ and Cl^- are 0.167 nm and 0.181 nm, respectively. Use this information to estimate the lattice constant for the conventional unit cell.

[7 marks]

1.2) Define the symbols in the Bragg Law, $n\lambda = 2\, d \sin\theta$.

A metal at 20 °C scatters a beam of monochromatic X-rays at a Bragg angle of 47.300°. When the specimen is heated to 220 °C this angle changes to 47.053°. Show that the coefficient of linear thermal expansion for the metal is 2×10^{-5} K^{-1}.

[7 marks]

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

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

[7 marks]

1.4) Sketch the density $g(E)$ of electron states as a function of energy E for a metal, as predicted by the free-electron theory. Which states are occupied at temperature T = 0 K? Estimate the fraction of the electrons which are thermally excited at room temperature in a metal with a Fermi energy of 5 eV.

[7 marks]

1.5) An electron is excited optically from the top of the valence band to the bottom of the conduction band in an indirect-gap semiconductor. Explain, with the aid of $E-k$ diagrams, what is meant by the each of the terms *phonon absorption* and *phonon emission* for the excitation.

[7 marks]

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

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

Note: For Ge the effective mass of the electrons is $m_e^* = 0.22\, m_e$, and the relative permittivity is $\varepsilon_r = 15.8$.

[7 marks]

1.7) Define the terms in the expression $E_y = RJ_xB_z$ for the *Hall Effect*, which applies for orthogonal geometry.

Calculate E_y for a metal specimen, with an electron concentration of 10^{29} m^{-3}, carrying a current density of 10^5 Am^{-2} and placed in a magnetic flux density of 0.5 T.

[7 marks]

1.8) What is meant by (a) the *critical temperature* T_c and (b) the *critical field* B_c for a type I superconductor. Sketch the relationship between B_c and temperature T for a typical type I superconductor.

Explain, briefly, the Silsbee hypothesis of critical currents.

[7 marks]

SECTION B – Answer TWO questions

2) Explain the meanings of the terms in the expression for the structure factor F_{hkl} in relation to the 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 body-centred cubic structure scatter X-rays only if $(h + k + l)$ is even.

[8 marks]

Tantalum has the body-centred cubic structure. Its atomic mass number is 181 and its density is 16660 kg m^{-3}.

A crystal of tantalum is placed in a monochromatic beam of X-rays of wavelength $\lambda = 0.15$ nm.

(a) Show that the lattice constant $a = 0.3304$ nm if the atoms are assumed to be hard spheres in close contact.

[6 marks]

(b) Show that the angle θ at which scattering is obtained from $(h\,k\,l)$ planes is given by $\sin^2\theta = (\lambda^2 / 4\,a^2)\,(h^2 + k^2 + l^2)$.

[5 marks]

(c) Calculate the angle at which the {220} reflection occurs.

[2 marks]

(d) Calculate the largest angle at which X-ray scattering will be observed.

[5 marks]

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

[4 marks]

At temperature *T*, the average energy of a quantum oscillator with angular frequency ω is given by

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

(a) Show that the Einstein expression for the heat capacity per mole may be written as

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

where θ_E is the Einstein temperature, ω_E is the Einstein frequency and $\theta_E = \hbar\omega_E / k_B$.

[8 marks]

(b) Discuss the behaviour of this expression at (i) high temperature and (ii) low temperature.

[6 marks]

(c) Discuss how the behaviour predicted from the Einstein expression compares with that observed experimentally. Explain, without derivation, the more realistic approach used by Debye to predict the temperature dependence of the heat capacity.

[4 marks]

(d) The variation of heat capacity with temperature for silicon can be fitted reasonably well using θ_E = 380 K. Use this information to calculate the zero-point energy for 1 kg of silicon. (The atomic mass number of silicon is 28.)

[8 marks]

4) Krönig and Penney showed that, in a one-dimensional crystal, electrons 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 $\alpha = m_e V/\lambda\hbar^2$, $\lambda = (2m_e E)^{½}/\hbar$, a is the period of the lattice, and V represents the strength of the potential barrier between the unit cells.

(a) Using a diagram, show how this relationship leads to a situation in which allowed energy bands are separated by forbidden energy bands.

[8 marks]

(b) Show further that when $V = 0$ (as in a metal) the solution reduces to the free-electron parabola $E = \hbar^2 k^2/2m_e$.

[7 marks]

(c) Draw a diagram, using the repeated zone scheme, to illustrate how the Krönig-Penney solutions are related to the free-electron parabola.

[6 marks]

(d) By considering the discontinuities that occur on such a diagram, explain how the energy gaps may be interpreted in terms of Bragg diffraction of the electron waves.

[9 marks]

5) Explain what is meant by an *intrinsic semiconductor*.

[3 marks]

For a semiconductor at temperature T the concentrations of electrons in the conduction band and holes in the valence band are respectively

$$n = AT^{3/2} \exp\left[\frac{-(E_g - E_F)}{k_B T}\right]$$

and $$p = BT^{3/2} \exp\left[\frac{-E_F}{k_B T}\right] ,$$

where E_g and E_F are the energy gap and Fermi energy, respectively, and A and B are constants.

Show that the intrinsic carrier concentration is

$$n_i = (AB)^{1/2} T^{3/2} \exp\left[\frac{-E_g}{2k_B T}\right]$$

[4 marks]

At temperatures above 275 K the energy gap of silicon is given by $E_g = E_0 - \alpha T$, where E_0 = 1.205 eV and $\alpha = 2.83 \times 10^{-4}$ eV K^{-1}. Show that the temperature coefficient of the intrinsic carrier concentration may be written as

$$\frac{1}{n_i}\frac{dn_i}{dT} = \frac{3}{2T} + \frac{E_0}{2k_B T^2} .$$

[8 marks]

Hence show that at 293 K the intrinsic carrier concentration increases by 10% for an increase in temperature of approximately 1.16 K.

[4 marks]

Use the original expression for n_i (with $E_g = E_0 - \alpha T$) to calculate the temperature at which the intrinsic carrier concentration is double the value at 293 K. (This will require an iterative technique.)

[8 marks]

Explain why an intrinsic semiconductor is not suitable for the majority of semiconductor device applications.

[3 marks]

FINAL PAGE