

King's College London

UNIVERSITY OF LONDON

This paper is part of an examination of the College counting towards the award of a degree. Examinations are governed by the College Regulations under the authority of the Academic Board.

B.Sc. EXAMINATION

CP/3402 Solid State Physics

Summer 2003

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.**

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

Boltzmann constant	$k_B = 1.381 \times 10^{-23} \text{ J K}^{-1} = 8.617 \times 10^{-5} \text{ eV K}^{-1}$
Planck constant	$h = 6.626 \times 10^{-34} \text{ J s}$
Reduced Planck constant	$\hbar = 1.055 \times 10^{-34} \text{ J s}$
Permeability of free space	$\mu_0 = 4\pi \times 10^{-7} \text{ H m}^{-1}$

SECTION A - Answer SIX parts of this section

- 1.1) Assuming the atoms are hard spheres, and stating any other assumptions needed, show that approximately 26 % of the close packed hexagonal structure is empty.

[7 marks]

- 1.2) Define the terms in the Bragg law for X-ray diffraction, $n\lambda = 2d \sin \theta$.

The two components of the K_α radiation from copper have a wavelength-separation of $\Delta\lambda = 0.38 \times 10^{-3} \text{ nm}$. For a certain crystal, with $d = 0.2325 \text{ nm}$, the angular separation of the two diffracted components when $n = 2$ is $\Delta\theta = 2.184 \times 10^{-3}$ radians. Calculate $\Delta\theta$ when $n = 3$.

[7 marks]

- 1.3) The relation between angular frequency ω and wavenumber k for waves propagating on a linear chain of atoms of mass M spaced a distance a apart is $\omega^2 M = 4K \sin^2(\frac{1}{2} ka)$, where K is the “spring constant.”

Sketch the dispersion curve of ω versus k . Obtain an expression for k when the group velocity is equal to half the velocity at which sound waves are propagated on the chain.

[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 $T = 0 \text{ K}$? 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) Explain what is meant by a *substitutional donor* in a group IV semiconductor.

The intrinsic carrier concentration for silicon at room temperature is $2 \times 10^{16} \text{ m}^{-3}$. Calculate the hole concentration for an n-type specimen of silicon containing an effective donor concentration of 10^{18} m^{-3} .

[7 marks]

- 1.6) Explain what is meant by a *direct gap semiconductor* and an *indirect gap semiconductor*. Give one example of each, and explain why direct gap materials are required to produce semiconductor lasers.

[7 marks]

- 1.7) The rectifier equation for the current I flowing through an ideal p-n junction at temperature T and forward bias V is $I = I_0[\exp(eV/k_B T) - 1]$.

Sketch this relationship for both negative and positive V , and define the meaning of the term I_0 . Explain why the behaviour of a real diode departs rapidly from the above expression for increasing positive values of V .

[7 marks]

- 1.8) Explain, briefly, the Silsbee hypothesis.

The type I superconductor mercury has a critical temperature $T_c = 4.2 \text{ K}$, and a critical field $B_c = 41.5 \text{ mT}$ at temperature $T = 0$. Calculate the critical current for a mercury wire of radius 1 mm at $T = 2 \text{ K}$.

[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 diffraction of X-rays from a crystalline solid:

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

[3 marks]

For a given angle of diffraction, on what does the parameter f_j principally depend?

[2 marks]

Describe the *sodium chloride* (NaCl) and *caesium chloride* (CsCl) crystal structures, and derive the *X-ray extinction rules* for each structure.

[13 marks]

When subjected to hydrostatic pressure, potassium chloride transforms from the NaCl structure to the CsCl structure at a well-defined pressure. At pressures just before the phase change the K–Cl bond length is 0.3053 nm, and just after the phase change the bond length is 0.3190 nm.

Show that the density of the KCl has increased by approximately 14 %.

In an X-ray diffraction experiment, in which hydrostatic pressure is applied to KCl, the intensity of the scattered X-rays is plotted versus the angle θ between the X-ray beam and the surface of the crystal. Just before the phase change occurred, the peak with the smallest angle of diffraction was observed at $\theta = 14.63^\circ$.

Show that, for pressures just after the phase change, the smallest-angle peak occurs at 17.22° .

[12 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]

How do the assumptions made by Debye differ from those made by Einstein?

[2 marks]

Sketch the form of the results obtained for both of these models (no mathematical derivation is required). What particular improvement in the results was obtained by the Debye model?

[7 marks]

At low temperatures T the Debye heat capacity C can be expressed in two

different ways: $C = \frac{12Nk_B\mathbf{p}^4}{5} \left(\frac{T}{\mathbf{q}_D} \right)^3$ or $C = \frac{2V\mathbf{p}^2k_B}{15} \left(\frac{1}{v_L^3} + \frac{2}{v_T^3} \right) \left(\frac{k_B T}{\hbar} \right)^3$.

Here v_L and v_T are the longitudinal and transverse velocities of sound, \mathbf{q}_D is the Debye temperature, and N is the number of atoms in a crystal of volume V .

Assume that v_L and v_T can be replaced by an average velocity v_{av} and obtain an expression for v_{av} in terms of N , V , \mathbf{q}_D and the fundamental constants.

[6 marks]

At low temperatures the temperature-dependence of the heat capacity of diamond can be fitted with $\mathbf{q}_D = 2220$ K. Use this information to calculate the average velocity of sound in diamond. The lattice constant of the cubic unit cell for diamond is $a = 0.3567$ nm.

[12 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

$$\cos(ka) = \cos(Ia) + \mathbf{a} \sin(Ia) ,$$

where $\mathbf{a} = m_e V / \hbar^2$, $I = (2m_e E)^{1/2} / \hbar$, 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

$$n = MA(m_e^*T)^{3/2} \exp\left[\frac{-(E_g - E_F)}{k_B T}\right] \quad \text{and} \quad p = A(m_h^*T)^{3/2} \exp\left[\frac{-E_F}{k_B T}\right],$$

where E_g and E_F are the energy gap and Fermi energy, respectively, and m_e^* and m_h^* are the effective masses for the electron and hole, respectively. M is a factor which depends on the number of conduction band minima, and $A = 5.557 \times 10^{66} \text{ K}^{-3/2} \text{ kg}^{-3/2} \text{ m}^{-3}$.

Show that the intrinsic carrier concentration is

$$n_i = M^{1/2} A(m_e^* m_h^*)^{3/4} T^{3/2} \exp\left[\frac{-E_g}{2k_B T}\right]$$

[4 marks]

At temperatures above 200 K the energy gap of germanium is given by $E_g = E_0 - \alpha T$, where α is a constant. Show that the temperature dependence of

the intrinsic carrier concentration may be written as $n_i = BT^{3/2} \exp\left[\frac{-E_0}{2k_B T}\right]$

where B is a constant. Hence, using the following data for germanium, plot a graph to determine E_0 and B :

T (K)	200	300	400	500	600	700	800	900
n_i (m^{-3})	5.8E15	2.0E19	1.4E21	1.9E22	1.2E23	4.3E23	1.4E24	2.7E24

[15 marks]

For Ge, $m_e^* = 0.22 m_e$, $m_h^* = 0.37 m_e$ and $M = 4$. Show that the energy gap at 300 K is 0.665 eV and that $\alpha \sim 4 \times 10^{-4} \text{ eV K}^{-1}$.

[8 marks]