# King's College London

#### UNIVERSITY OF LONDON

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**B.Sc. EXAMINATION** 

**CP3402 Solid State Physics** 

Summer 2004

Time allowed: THREE Hours

Candidates should answer no more than SIX parts of SECTION A, and no more than TWO questions from SECTION B.

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.

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## **Physical Constants**

| Permittivity of free space       | $\boldsymbol{\varepsilon}_0 =$ | $8.854 \times 10^{-12}$ | $F m^{-1}$                |
|----------------------------------|--------------------------------|-------------------------|---------------------------|
| Permeability of free space       | $\mu_0 =$                      | $4~\pi\times10^{-7}$    | $H m^{-1}$                |
| Speed of light in free space     | c =                            | $2.998 \times 10^{8}$   | $m s^{-1}$                |
| Gravitational constant           | G =                            | $6.673 \times 10^{-11}$ | $N m^2 kg^{-2}$           |
| Elementary charge                | e =                            | $1.602 \times 10^{-19}$ | C                         |
| Electron rest mass               | $m_{\rm e}$ =                  | $9.109 \times 10^{-31}$ | kg                        |
| Unified atomic mass unit         | $m_{\rm u} =$                  | $1.661 \times 10^{-27}$ | kg                        |
| Proton rest mass                 | $m_{\rm p}~=$                  | $1.673 \times 10^{-27}$ | kg                        |
| Neutron rest mass                | $m_{\rm n} =$                  | $1.675 \times 10^{-27}$ | kg                        |
| Planck constant                  | h =                            | $6.626 \times 10^{-34}$ | J s                       |
| Boltzmann constant               | $k_{\mathrm{B}} =$             | $1.381 \times 10^{-23}$ | $J K^{-1}$                |
| Stefan-Boltzmann constant        | $\sigma$ =                     | $5.670 \times 10^{-8}$  | $W\ m^{-2}\ K^{-4}$       |
| Gas constant                     | R =                            | 8.314                   | $J \; mol^{-1} \; K^{-1}$ |
| Avogadro constant                | $N_{\rm A} =$                  | $6.022 \times 10^{23}$  | $\text{mol}^{-1}$         |
| Molar volume of ideal gas at STP | =                              | $2.241 \times 10^{-2}$  | $m^3$                     |
| One standard atmosphere          | $P_0 =$                        | $1.013 \times 10^{5}$   | $N m^{-2}$                |

## SECTION A – Answer SIX parts of this section

1.1 Describe the sodium chloride (NaCl) crystal structure. Explain why NaF, which has the NaCl structure, scatters X-rays as though its structure were simple cubic.

[7 marks]

1.2 Define the terms in the Bragg law  $n\lambda = 2d\sin\theta$ . Derive an expression for the small change in  $\theta$  produced by a small change in  $\lambda$ . Hence show that for  $\theta = 85^{\circ}$  a 0.1 % change in  $\lambda$  produces a change in  $\theta$  of approximately 0.7°.

[7 marks]

1.3 The cut-off frequency for the vibrations of a one-dimensional chain of identical atoms is  $\omega_c = 2(K/M)^{\frac{1}{2}}$ . Define the terms in this expression. Assuming that an expression of this type also applies to a three-dimensional crystal, show that the cut-off frequency for  $^{30}$ Si is 3.4 % lower than that for  $^{28}$ Si.

[7 marks]

1.4 The Einstein expression for the heat capacity C of a non-metallic crystalline solid at temperature T is given by

$$C = 3N_{\rm A}k_{\rm B}\left(\frac{\theta_{\rm E}}{T}\right)^2\frac{\exp(\theta_{\rm E}/T)}{\left[\exp(\theta_{\rm E}/T)-1\right]^2}$$
, where  $\theta_{\rm E}$  is the Einstein temperature.

Show that, for  $\theta_E = 300$  K, the heat capacity has reached approximately half of its maximum value by T = 100 K.

[7 marks]

1.5 The resistivity  $\rho$  of a metal is given by  $\rho = \frac{m_e}{ne^2\tau}$ , where n is the electron concentration and  $\tau$  is the relaxation time. By considering the behaviour of  $\tau$ , show how *Matthiessen's rule* is obtained.

[7 marks]

1.6 Two of the valence bands in silicon are degenerate at k = 0. Show this information on a sketch of E vs. k, where E is the energy and k is the wavenumber. Identify, giving an explanation, the *heavy hole band* and the *light hole band*. You may assume that

electrons moving in a periodic potential have an effective mass 
$$m_{\rm e}^* = \hbar^2 \left(\frac{{\rm d}^2 E}{{\rm d}k^2}\right)^{-1}$$
.

[7 marks]

- 1.7 Stating any assumptions, calculate the room-temperature hole concentration for an n-type specimen of silicon containing an effective donor concentration of  $10^{18}$  m<sup>-3</sup>. (The intrinsic carrier concentration for silicon at room temperature is  $2 \times 10^{16}$  m<sup>-3</sup>.)
- 1.8 The rectifier equation for the current I flowing through an ideal p-n junction at temperature T and forward bias V is  $I = I_0[\exp(eV/k_BT) 1]$ .

Define the meaning of the term  $I_0$ . For a real rectifier diode, explain what is meant by the *forward dynamic resistance*. A silicon rectifier has  $I_0 = 10^{-10}$  A at room temperature (293 K), and a forward dynamic resistance of 0.2  $\Omega$ . Calculate the voltage across the whole device for a forward current of 1 A.

[7 marks]

## **SECTION B – Answer TWO questions**

2. (a) 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:

$$F_{hkl} = \sum_{j} f_{j} \exp \{2\pi i (h x_{j} + k y_{j} + l z_{j})\}.$$

[5 marks]

- (b) Show that, for allowed diffractions,
  - (i) for the body centred cubic (BCC) structure (h + k + l) must be even
  - (ii) for the face centred cubic (FCC) structure, h, k and l must be all odd or all even.

[12 marks]

(c) X-ray diffraction measurements from a polycrystalline sample, known to be either BCC or FCC, gave diffractions at the following angles, using X-rays with wavelength 0.175 nm.

Angles (degrees): 24.8, 29.0, 43.3, 53.5, 57.1, 75.8.

From these data, and the results of part (b), determine the crystal structure and the lattice constant.

[13 marks]

3. (a) In the Debye analysis for the heat capacity of a non-metallic crystalline solid, the lattice vibration energy at temperature *T* is given by

$$E = E_Z + \frac{9N_A}{\omega_D^3} \int_0^{\omega_D} \frac{\hbar \omega^3 d\omega}{[\exp(\hbar \omega / k_B T) - 1]} \quad \text{mol}^{-1}$$

where  $E_Z$  is the zero-point energy,  $\omega_D$  is the Debye frequency and  $\omega$  is the frequency of a lattice mode.

Show that the heat capacity at low temperatures is given by

$$C = \frac{12N_{\rm A}k_{\rm B}\pi^4}{5} \left(\frac{T}{\theta_{\rm D}}\right)^3 \text{ mol}^{-1}$$
 where  $\theta_{\rm D}$  is the Debye temperature.

[10 marks]

You may assume that  $\int_{0}^{\infty} \frac{x^4 e^x dx}{(e^x - 1)^2} = \frac{4\pi^4}{15}.$ 

(b) Explain what is meant by the Fermi energy of a metal. Sketch the distribution of occupied energy levels at T = 0 and at T > 0.

The density-of-states function at the Fermi energy  $E_{\rm F}$  is given by  $g(E_{\rm F}) = \frac{3N_{\rm A}}{2E_{\rm F}}$ .

Show that the heat capacity of the free electrons in a metal is given approximately by

$$C_V = \frac{3}{2} N_A k_B \frac{T}{T_E} \text{ mol}^{-1}$$
 where  $T_F$  is the Fermi temperature.

[10 marks]

(c) The molar heat capacity  $C_V$  of tungsten at low temperatures T has the following values:

$$T(K)$$
 1 2 3 4 10  $C_V(\text{mJ K}^{-1} \text{ mol}^{-1})$  1.36 2.90 4.82 7.23 43

By plotting a suitable graph, determine the Debye temperature and an approximate value of the Fermi energy (in eV).

[10 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 a is the period of the lattice,  $\lambda = \frac{(2m_{\rm e}E)^{1/2}}{\hbar}$ ,  $\alpha = \frac{m_{\rm e}V}{\lambda \hbar^2}$  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.

[10 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) Using the results from the Krönig-Penney model, for a crystal with atoms separated by  $3 \times 10^{-10}$  m, and a potential barrier of strength  $V = 2 \times 10^{-9}$  eV m, show that electrons of energy 15 eV will lie in an allowed band.

[13 marks]

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

$$n = MA(m_{\rm e}^*T)^{3/2} \exp\left[\frac{-(E_{\rm g} - E_{\rm F})}{k_{\rm B}T}\right]$$
 and  $p = A(m_{\rm h}^*T)^{3/2} \exp\left[\frac{-E_{\rm F}}{k_{\rm B}T}\right]$ ,

where  $E_{\rm g}$  and  $E_{\rm F}$  are the energy gap and Fermi energy, respectively, and  $m_{\rm e}^*$  and  $m_{\rm h}^*$  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 is a constant.

(a) Explain what is meant by an *intrinsic semiconductor*.

[3 marks]

(b) For intrinsic germanium the mobilities of the electrons and holes are both approximately proportional to  $T^{-3/2}$ . Show that the electrical conductivity is given approximately by  $\sigma = C \exp \left[ \frac{-E_g}{2k_B T} \right]$  where C is a constant.

[8 marks]

(c) At temperatures above 200 K the energy gap of germanium in eV is given by  $E_{\rm g} = 0.782 - \alpha T$ , where  $\alpha$  is a constant. Use the expression in (b) to calculate the temperature at which the conductivity of intrinsic germanium is a factor of 10 higher than its value at 293 K.

[12 marks]

(d) Explain, without mathematical derivation, how the addition of a modest concentration of a substitutional group V impurity atom to germanium or silicon leads to a situation in which the electron concentration is almost constant over a range of temperatures.

[7 marks]