One hour thirty minutes

A list of Constants is enclosed

UNIVERSITY OF MANCHESTER

Fundamentals of Solid State Physics

4 June 2019, 2:00 – 3:30

Answer **ALL** parts of question 1 and **TWO** other questions

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Electronic calculators may be used, provided that they cannot store text.

The numbers are given as a guide to the relative weights of the different parts of each question.

P.T.O.

1.

a) Using a molecular orbital energy level diagram, explain why the bond length of the H_2^+ molecular ion is larger than that of the H_2 molecule. State whether you expect the bond length for the three-electron species H_2^- to be smaller or larger than that for H_2. Briefly justify your answer.

[5 marks]

b) The density of free electrons n in a metal is given by

$$n = \int_0^\infty g(\varepsilon) f(\varepsilon, T) \mathrm{d}\varepsilon,$$

where $g(\varepsilon)$ is the density of states function and $f(\varepsilon, T)$ is the Fermi-Dirac occupation function.

Explain why this expression can be written as

$$n = \int_0^{\varepsilon_\mathrm{F}} g(\varepsilon) \mathrm{d}\varepsilon,$$

where ε_F is the Fermi energy. Hence show that

$$n = A{\varepsilon_\mathrm{F}}^{3/2},$$

where A is a constant.

[5 marks]

c) Use the Drude model to derive an expression for the electrical conductivity of a metal, defining the terms you use.

[5 marks]

d) Sketch the dispersion relation $\varepsilon(k)$ for a nearly free electron interacting with a one-dimensional lattice, over the range $-\frac{2\pi}{a} \leq k \leq +\frac{2\pi}{a}$, where a is the spacing of the atoms.

[5 marks]

e) Using a diagram, show the experimental arrangement used in a Hall-effect measurement. By considering the forces on electrons in a current-carrying conductor, show that the Hall coefficient R_H is given by

$$R_\mathrm{H} = -\frac{1}{ne},$$

where n is the electron density and e is the electronic charge.

[5 marks]

P.T.O.

2.

a) Briefly describe each of the following, including its origin and its influence on the bonding of solids. In each case give one specific example, and discuss how it affects the interatomic distance in a solid:

(i) covalent bonding;

(ii) dipole-dipole interaction.

[6 marks]

b) Describe the two-dimensional primitive unit cell of graphene. State the type of lattice formed and the basis. Draw one unit cell.

[4 marks]

c) Three-dimensional graphite is made up of sheets of the two-dimensional material described in part b). X-ray diffraction is used to measure the distance between adjacent rows of carbon atoms in the layers, and the distance between the two-dimensional sheets.

(i) Draw diagrams to show how a single-crystal sample of graphite must be orientated with respect to the incident and scattered beams in order to make each of these measurements.

[2 marks]

(ii) The wavelength of the X-rays is 1.54 Å, and peaks are found at scattering angles of 42.4° and 26.6° in first order. Calculate the nearest-neighbour distance in the sheet, and the distance between the sheets.

[4 marks]

(iii) State the effects that give rise to the binding in the sheets, and to the binding between the sheets in graphite.

[2 marks]

d) Briefly describe how the Tight-Binding Model may be used to model the electronic structure of graphene close to the Fermi energy. Draw an E-k diagram of the band dispersion at the K-point of the Brillouin zone, indicate the band filling, and mark the position of the Dirac point. Indicate the position of the Fermi energy for the three cases of perfect undoped graphene, n-type doping and p-type doping.

[7 marks]

P.T.O.

3.

a) Define the terms ‘intrinsic semiconductor’ and ‘extrinsic semiconductor’.

[2 marks]

b) The electron density n in the conduction band of an *intrinsic* semiconductor can be written as

$$n = N_C e^{\frac{-(E_C-\varepsilon_F)}{k_B T}},$$

where N_C is the effective density of states in the conduction band, and all other symbols have their conventional meaning.

Calculate n at a temperature of 300 K for GaN, given that the band gap is 3.2 eV and the value of N_C is 4 x 10^{25} m^{-3}.

[3 marks]

c) Sketch a graph showing a typical variation of log(n) where n is the free electron concentration for an n-type semiconductor as a function of the inverse of the absolute temperature. Indicate three important ranges on your graph and explain why the different ranges exist.

[6 marks]

d) Extrinsic n-type doping can be achieved in GaN by substituting silicon (Si) atoms onto Ga lattice sites. Draw a schematic energy level diagram to illustrate the band structure at T = 0 K of GaN doped with Si atoms. Mark on your diagram the positions of the conduction and valence band edges and the Fermi energy.

[5 marks]

e) The dopant ionisation energy in Si-doped GaN is 20 meV. Assuming the semiconductor is in the impurity range, estimate the carrier density due to the dopant atoms at 300 K. You may use the value of N_C given in part b). Compare your answer with your answer to part b), and give a physical interpretation.

[5 marks]

f) Comment on the suitability of GaN in the following applications:

(i) as a transistor;

[2 marks]

(ii) as a light-emitting diode.

[2 marks]

P.T.O.

4.

a) Sketch a graph of the measured molar heat capacity at constant volume, C_V, *versus* absolute temperature for copper, which has an Einstein temperature of 276 K.

[3 marks]

b) State the law of equipartition of energy. Using this and the first law of thermodynamics show for a monovalent solid that C_V is equal to $3R$ where R is the universal gas constant.

[6 marks]

c) Describe the Einstein model of specific heat, and explain why it predicts that C_V should depend on temperature as opposed to the prediction based on the equipartition of energy. In your answer briefly discuss the relevance of the Einstein temperature.

[6 marks]

d) Using the Einstein model, calculate the energy difference between the allowed vibrational states in copper.

[2 marks]

e) Using the classical free electron model, estimate the contribution to the molar specific heat provided by *free electrons* in a metal.

[3 marks]

f) Explain qualitatively why, taking into account the quantum nature of the free electrons in a metal, your prediction in part e) is not reflected in your graph in part a) for $T \sim 300$ K.

[5 marks]

END OF EXAMINATION PAPER