ONE HOUR THIRTY MINUTES

A list of constants is enclosed.

UNIVERSITY OF MANCHESTER

Fundamentals of Solid State Physics

32nd May/June 2023, xx - xx

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.

1. a) What is the Born-Oppenheimer approximation for molecules? Why is it a valid approximation?

[3 marks]

b) Write down an expression for the Coulomb integral in the molecular-orbital theory of H_2^+. Explain any notation you use.

[4 marks]

c) The electronic configuration of a magnesium atom is [Ne]$(2s)^2$. Explain, with the aid of a sketch for the energy band structure in the nearly-free electron model, why solid magnesium shows metallic conductivity.

[5 marks]

d) Write down a model potential for the pair-wise interaction between ions of an ionic solid. Explain the physical origin of each term.

[4 marks]

e) i) Given that the phonons in a 3D monatomic solid can be represented by a plane wave of form, $e^{i\mathbf{k}\cdot\mathbf{r}}$, show that the density of states for the phonons is related to their energy by

$$g(E) \propto E^2,$$

where the phonon energy $E = \hbar v_p k$ and v_p is the speed of sound.

[5 marks]

ii) Consider a mole of this monatomic solid for which the density of states for the phonons is written as $g(E) = AE^2$. Find the constant A in terms of the Debye temperature Θ_D and the gas constant R.

[4 marks]

2. a) i) The molar volume of sodium is 23.8×10^{-6} m^3, the electron mobility at room temperature is $5.3 \times 10^{-3}\,\mathrm{m^2V^{-1}s^{-1}}$, and the atomic electronic configuration is [Ne]$(3s)^1$. Estimate the value of the electrical conductivity of sodium at room temperature.

[5 marks]

ii) Estimate also the value of the electronic thermal conductivity of sodium at room temperature. You may assume the following value for the Lorenz number

$$L_D \approx 1.67 \times 10^{-8}\,\mathrm{W\Omega K^{-2}}.$$

[3 marks]

b) An electron moving in a 1D solid of lattice constant a is described by a Hamiltonian $\hat{H}$. A crystal orbital of the electron is given by

$$\psi_k = \sum_n e^{ikna}\phi_n(x),$$

where n is summed over all lattice sites, k is the wavenumber, ϕ_n is the atomic orbital at site n.

i) Using the tight-binding approximation, show that the energy spectrum of the electron is given by

$$E(k) = \alpha + 2\beta\cos(ka),$$

and find the expressions for α and β as integrals involving $\hat{H}$.

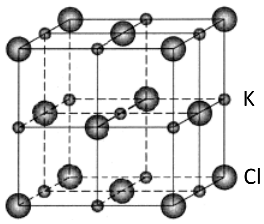
[10 marks]

ii) State the physical meanings of α and β. Given that β is always negative, sketch $E(k)$ for $-\pi/a < k < \pi/a$. Discuss the nature of bonding contributed by the electron in the limits $k \to 0$ and $k \to \pm\pi/a$.

[7 marks]

3. a) KCl has the following crystal structure. State the nature of bonding in the solid and the Bravais lattice type. How many atoms are there in the basis?

[6 marks]



b) How many acoustic and optical vibrational branches (modes per basis) are there in a KCl crystal?

[3 marks]

c) An X-ray experiment, using a wavelength of 1.54 Å, measures the first-order scattering from (200) planes of a KCl crystal at a scattering angle of 28.4°.

i) Sketch the experimental arrangement, showing the alignment of the (200) plane in the unit cell, and the incident and scattered X-ray beams.

[4 marks]

ii) Calculate the (200) interplanar distance. What is the value of the lattice parameter of the conventional unit cell?

[7 marks]

iii) Calculate mass density of KCl, given the atomic mass is 39.1 u for K and 35.4 u for Cl.

[5 marks]

4. a) i) State the law of equipartition of energy. What does this predict for the molar heat capacity of a monatomic solid?

[4 marks]

ii) Sketch the form of a typical experimental plot of the molar heat capacity C_V as a function of temperature, from absolute zero to room temperature. Explain the limiting value of C_V at absolute zero.

[5 marks]

b) i) The electron density in the conduction band of a semiconductor at temperature T is given by

$$n = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2} \exp\left(\frac{E_F - E_C}{k_B T}\right),$$

where m_e^* is the electron effective mass, E_F the Fermi energy, and E_C the energy of the conduction band edge. Making a simplifying assumption that the effective masses of electrons in the conduction band and of holes in the valence band of Ge are both equal to $0.1 m_e$ and the energy gap $E_G = 0.7$ eV, calculate the hole density in the valence band of intrinsic Ge at 1000 K.

[6 marks]

ii) Germanium ($Z = 32$) is doped by substituting arsenic (As, $Z = 33$) atoms. Identify the type of doping. Sketch an energy-level diagram to illustrate the band structure at $T = 0$ K of Ge doped with As atoms. Mark on your diagram the positions of the conduction and valence band edges and the Fermi energy.

[5 marks]

iii) The dopant ionization energy in As-doped Ge is 5.5 meV. Assuming the semiconductor is in the impurity range with impurity density 10^{25} m^{-3}, estimate the carrier density of the semiconductor at 300 K. Use your answers in (i) and (iii) to comment on the properties of the doped and intrinsic Ge.

[5 marks]

END OF EXAMINATION PAPER