<u>ONE HOUR THIRTY MINUTES</u>

A list of constants is enclosed.

UNIVERSITY OF MANCHESTER

Fundamentals of Solid State Physics

32nd May/June 2022, xx - xx

Answer **<u>ALL</u>** parts of question 1 and **<u>TWO</u>** other questions

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) Write down $2s\sigma$ and $2s\sigma^*$ molecular orbitals for diatomic molecules in terms of suitable atomic orbitals and explain any notation you use. Which of the two molecular orbitals has lower energy and why?

[5 marks]

b) Solid tungsten has a body-centered cubic crystal structure with one atom in the basis. Sketch its conventional unit cell. How many atoms are there in the cell? What is the number of nearest-neighbours of an atom in the solid? Why is the conventional unit cell often used rather than the primitive unit cell?

[5 marks]

c) Given that the Fermi energy of solid tungsten is 9.75 eV, determine the free electron density in the solid. Given that solid tungsten has mass density of 19.3 $\mathrm{g/cm^3}$ and an atomic weight of 183.84, calculate the number of free electrons each tungsten atom contributes.

[6 marks]

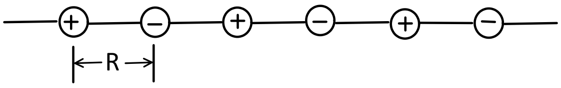
d) List three types of bonding in solids. State the main nature of each bonding and give an example of solids for each bonding.

[6 marks]

e) At room temperature, a sample of intrinsic germanium has a free electron concentration of $2.33 \times 10^{19}\ \mathrm{m^{-3}}$. The electron and hole mobilities are $0.39\,\mathrm{m^2V^{-1}s^{-1}}$ and $0.19\,\mathrm{m^2V^{-1}s^{-1}}$ respectively. Calculate the conductivity of this sample.

[3 marks]

2. a) An infinitely long one-dimensional (1D) solid consists of alternating positive and negative ions, with charge $+e$ and $-e$, and mass m_+ and m_-, respectively, as shown in the following diagram. The nearest neighbour separation is R.



i) In addition to the Coulomb interactions between the ions, there is a short-range repulsion between the nearest neighbours only described by the potential, $U = A/R^9$, with positive parameter A. Determine the total potential energy per unit cell of the 1D solid. Derive an expression for the equilibrium separation R in terms of A and other parameters of the potentials.

You may find the following summation useful

$$\ln 2 = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \cdots .$$

[6 marks]

ii) Given that the vibrational motion in a 1D solid can be modeled by considering the bonds as springs with a spring constant K, write down the equations for the displacements of the ions in a basis (but do not solve them) and explain any notation you use.

[3 marks]

There are two vibrational modes in the solid with the spectra $\omega(k)$ given by

$$\omega^2 = \frac{K}{\mu} \pm K\sqrt{\frac{1}{\mu^2} - \frac{4}{m_- m_+}\sin^2(kR)}, \quad \text{where}\, \mu = \frac{m_- m_+}{m_- + m_+}.$$

Which of these modes is acoustic and which is optical? Find the expressions of ω of the two modes in the limits $k \to 0$. Determine the sound velocity in terms of the spring constant K. Describe briefly the motion of the ions in the basis in the limit $k \to 0$ for the two modes.

[6 marks]

b) i) Write down the electronic configuration for C_2 and determine its bond order. After removing one electron, will the molecular ion C_2^+ have a shorter or longer bond length? Explain why.

[5 marks]

ii) Molecular C_2 can absorb light of wavelength 515 nm and has a bond length of 1.24 Å. Determine the electronic and rotational excitation energies of C_2 in eV. From your value of the electronic excitation energy, estimate the vibrational energy-level interval of C_2 in eV.

[5 marks]

3. a) i) Find the density of states $g(E)$ for free electrons in a metal. Derive an expression for the Fermi energy E_F in terms of the electron concentration n.

[7 marks]

ii) The free electron density of copper is $n = 8.5 \times 10^{28}$ m^{-3}. Calculate its Fermi velocity v_F and Fermi temperature T_F. Describe the significance of this value of T_F.

[6 marks]

b) i) Use the Drude model to derive the electronic conductivity of a metal in terms of the electron density n and collision time τ.

[3 marks]

ii) Describe what really happens for the electric resistivity in metals in terms of collisions. Sketch the resistivity as a function of temperature and describe the general behaviours of resistivity in different regions of temperature.

[6 marks]

iii) Calculate the drift velocity v_D of copper with the electron concentration given in (a.ii) for a current density of 10^8 Am^{-2}. Compare the value of v_D with your value of Fermi velocity v_F in (a.ii) and comment on what happens to the Fermi sphere of copper when such a current flows.

[3 marks]

4. a) i) Without using formulae or diagrams, describe the main features of electric conductivity in intrinsic silicon. Describe what happens to the conductivities after doping with phosphorous atoms, and with boron atoms.

[7 marks]

ii) The electron and hole mobilities in silicon are $0.12\,\mathrm{m^2V^{-1}s^{-1}}$ and $0.05\,\mathrm{m^2V^{-1}s^{-1}}$ respectively. Two samples of silicon are doped, one with phosphorous atoms of concentration $7.5\times10^{21}\ \mathrm{m^{-3}}$, and the other with boron atoms of concentration $1.6\times10^{20}\,\mathrm{m^{-3}}$. Assuming that all dopant atoms are ionized, calculate the conductivity in each case. You can ignore the intrinsic conductivity of silicon.

[4 marks]

b) i) Neon forms an fcc solid. Write down the pairwise potential between neon atoms, and state the origin of each term in the potential.

[4 marks]

ii) X-rays of wavelength 1.54 Å are used in a diffraction measurement of the inter-layer distance between (101) planes in solid neon. Sketch the experimental arrangement, showing the relationship between the alignment of the conventional cubic unit cell and the incident and scattered x-ray beams. Mark the scattering angle in your sketch.

[3 marks]

iii) The (101) planes diffract x-rays in first order with a scattering angle of 28.5°. Calculate the inter-layer (101) distance. Determine the lattice constant of the cubic unit cell. What is the nearest-neighbour distance between neon atoms?

[7 marks]

END OF EXAMINATION PAPER