ONE HOUR THIRTY MINUTES

A list of constants is enclosed.

UNIVERSITY OF MANCHESTER

Fundamentals of Solid State Physics

[redacted] 2024, [redacted]

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

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The use of calculators is permitted, as long as they cannot store text and have no graphing capability.

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

1. a) What is a typical value of the lattice constant of a crystal? Give reasons for your answer.

[4 marks]

b) List all the 5 Bravais lattices in 2D. Which Bravais lattice does a honeycomb lattice belong to? Sketch the honeycomb lattice and its primitive unit cell.

[6 marks]

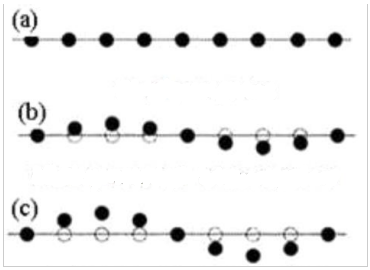
c) Write down expressions for $2p\sigma$ and $2p\sigma*$ molecular orbitals. Explain any notation you use.

[5 marks]

d) i) Define phonons in a lattice.

[2 marks]

ii) The following diagrams show vibrational states of a 1D lattice.



What is the number of phonons in (a)?
The vibrations in (b) and (c) have the same frequency. Which has the greater number of phonons and why?

[4 marks]

e) For a sample of intrinsic gallium arsenide at room temperature, the conductivity is $1.0 \times 10^{-6}\ \Omega^{-1}\mathrm{m}^{-1}$, the electron and hole mobilities are, respectively 0.85 and 0.04 $\mathrm{m}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$. Calculate the electron and hole densities.

[4 marks]

2. a) i) Write down an expression for the exchange integral in the molecular-orbital (MO) theory of H_2^+. Explain any notation you use.

[5 marks]

ii) Sketch the energy of H_2^+ in the bonding MO as a function of the separation between the two protons. Identify the dissociation energy and bond length of the molecule in your sketch.

[5 marks]

b) i) Consider a linear chain of identical atoms of mass M and lattice constant a, where the forces between nearest neighbours and next-nearest neighbours are included. Take the spring constants for the nearest-neighbour and next-nearest-neighbour interactions to be S_1 and S_2 respectively. Show that the dispersion relation, $\omega(k)$, for lattice vibrations of the chain is given by

$$M\omega^2 = 2S_1[1 - \cos(ka)] + 2S_2[1 - \cos(2ka)].$$

[8 marks]

ii) By considering the limit $ka \ll 1$, find the speed of sound in the 1D lattice. You may find the following expansion useful

$$\cos x = 1 - \frac{1}{2}x^2 + \cdots, \quad \text{for } x \ll 1.$$

[4 marks]

iii) What is the largest energy of a phonon in the 1D lattice?

[3 marks]

3. a) The electron density of iron is 1.7×10^{29} m^{-3}. Calculate the Fermi energy and Fermi temperature of iron. Discuss briefly the physical implications of this Fermi temperature.

[6 marks]

b) The valence electrons in a calcium atom are in the shell $(4s)^2$. Describe, with the aid of a sketch for the density of states as a function of energy, how the nearly-free electron model is modified to account for the metallic conductivity of solid calcium.

[4 marks]

c) The calcium atoms are arranged in a face-centred cubic lattice. An X-ray experiment, using a wavelength of 1.54 Å, measures the first-order scattering from (200) planes of the crystal at a scattering angle of 32.2°.

i) Sketch a conventional unit cell, 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 and determine the lattice constant. What is the value of the nearest-neighbour distance between two calcium atoms?

[6 marks]

iii) Calculate the mass density of solid calcium, given that the atomic mass of calcium is 40.1 u.

[5 marks]

4. a) i) Write down the ground-state electronic configuration of the molecular ion O_2^+ and calculate its bond order. Will this ion have shorter or longer bond length than O_2? Explain your answer.

[5 marks]

ii) An O_2 molecule absorbs light of wavelength 145 nm. Determine its electronic energy in eV. Estimate its vibrational and rotational energies in eV.

[6 marks]

b) Define a hole in a semiconductor and give its charge.

The energy spectrum of an electron in a valence band of a semiconductor is given by

$$E(k) = -Ak^2,$$

where $A = 2.0 \times 10^{-38}$ Jm^2. Calculate the effective mass of the electron in terms of electron mass m_e.

A hole is created in the valence band. Determine its effective mass.

[6 marks]

c) i) Write down the expression for the donor binding energy ΔE as measured from the conduction band edge for a doped semiconductor and explain any notation you use.

[3 marks]

ii) For the semiconductor Indium phosphide (InP), the effective electron mass $m_e^* = 0.08m_e$ and the relative permittivity $\epsilon = 12.4$. Calculate the absolute value of the donor binding energy for electrons doped into InP. Comment on the implication of your results on the conductivity given that the bandgap of InP is 1.5 eV.

[5 marks]

END OF EXAMINATION PAPER