

Answer EVERY question from section A and TWO questions from section B.

The numbers in square brackets in the right-hand margin indicate the provisional allocation of maximum marks per sub-section of a question.

Mass of the electron	m_e	=	9.11×10^{-31}	kg
Charge on the electron	e	=	-1.602×10^{-19}	C
Permittivity of free space	ϵ_0	=	8.854×10^{-12}	F m ⁻¹
Boltzmann's constant	k_B	=	1.38×10^{-23}	J K ⁻¹
Planck's constant/ 2π	\hbar	=	1.05×10^{-34}	J s

SECTION A

[Part marks]

1. Draw a sketch showing the three-dimensional arrangement of lattice points in the *body centred cubic* (BCC) lattice. How many nearest neighbours surround each lattice point? [3]

If a BCC lattice is filled with touching spheres, what fraction of space lies inside the spheres? [4]

2. The Lennard-Jones (LJ) potential is used to model the interaction between two atoms of inert gas separated by a distance, R ,

$$U(R) = 4\epsilon \left[\left(\frac{\sigma}{R} \right)^{12} - \left(\frac{\sigma}{R} \right)^6 \right].$$

What is the physical mechanism underlying each of the two terms? [3]

For an isolated pair of atoms interacting by this LJ potential, determine their equilibrium separation. [3]

3. Sketch a typical wavefunction of electrons inside a metal crystal that justifies the use of the free electron approximation, even when a strong influence of the ion cores is present. [3]

Draw a detailed diagram showing how the filling of states in a free-electron metal changes when an electric field is applied. What mechanism is responsible for maintaining a steady state configuration? [4]

4. A piece of monovalent metal, such as sodium, contains N atoms within a volume V . Use the free-electron gas model to derive the Fermi energy, which is the energy of the highest-lying occupied electronic state relative to the lowest. [4]
Explain how this energy is responsible for the metallic cohesion of sodium. [3]
5. Sketch the arrangement of electron bands near the Fermi level of a semiconductor, indicating which bands are (mostly) filled and which are (mostly) empty. Be sure to label the axes and bands. [3]
Use your diagram to explain the dominant influence of temperature on the concentration of “holes” in an undoped semiconductor. [4]
6. Describe with the aid of a suitable diagram how a “p-channel” field-effect transistor can be made by suitable doping of a block of silicon. [4]
Explain briefly how the device can be used to amplify an electrical signal. [2]

SECTION B

7. The energy of an electron within a band as a function of its wavevector is given by the tight-binding expression (in one dimension),

$$E(k) = -\alpha - \gamma \sum_m \exp(-ik\rho_m)$$

where γ is given by the integral expression

$$\gamma = - \int \phi^*(x - \rho) \mathcal{H} \phi(x) dx.$$

- (a) Explain the meaning of all the symbols represented in these expressions. What is the range of the sum and integral? [8]
- (b) What is the corresponding expression for α in terms of the same symbols? [6]
- (c) Evaluate the integral γ for the following wavefunction, assuming it is an eigenstate of the Hamiltonian, being careful to distinguish the cases $x_0 \leq 2\rho$ and $x_0 > 2\rho$: [8]

$$\begin{aligned} \phi(x) &= \sqrt{\frac{1}{2x_0}} & |x| \leq x_0 \\ \phi(x) &= 0 & |x| > x_0 \end{aligned}$$

- (d) Hence evaluate the energy of an electron in a linear chain of these atoms with a spacing a and make a graph of the result for the two cases $x_0 \leq 2a$ and $x_0 > 2a$. [8]

8. This question refers to the one-dimensional phonon dispersion relation.

- (a) Show, with the aid of a suitable diagram, the difference between how the atoms move in a *longitudinal* and *transverse* acoustic mode of vibration of a crystal lattice. [6]
- (b) Derive an expression for the allowed frequencies of longitudinal waves in a one-dimensional chain of identical atoms, each of mass M , spaced a apart, connected by springs of force constant C as a function of the wavevector K . [10]
- (c) Show by substitution that the frequencies corresponding to $K = \frac{\pi}{a} \pm \Delta k$ are the same. [8]
- (d) Demonstrate, with the aid of a suitable diagram, that the positions of the atoms at all times corresponding to $K = \frac{\pi}{a} \pm \Delta k$ are also the same. [6]

9. Powder specimens of three different monoatomic cubic crystals are analysed with X-ray diffraction (wavelength 1.5 Å). It is known that one sample is simple cubic (sc), one is face-centered cubic (fcc) and one has the diamond structure (diamond). The approximate positions (2θ) of the first four peaks in each case are:

A		B		C	
2θ	$\sin^2 \theta$	2θ	$\sin^2 \theta$	2θ	$\sin^2 \theta$
42.2°	0.130	28.8°	0.062	42.8°	0.133
49.2°	0.178	41.0°	0.123	73.2°	0.355
72.0°	0.345	50.8°	0.184	89.0°	0.491
87.3°	0.476	59.6°	0.247	115.0°	0.711

For later convenience, the corresponding $\sin^2 \theta$ have also been given.

(a) Why is diffraction only seen at these angles and not in between? State the law that connects the Bragg angle θ and the spacing between the lattice planes, and relate it to the reciprocal lattice vector \vec{G} . [7]

(b) Consider the fcc lattice as an sc lattice with a 4-atom basis and the diamond lattice as an fcc lattice with a basis $\{0, 0, 0\}$, $\{\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\}$, where a is the side of the conventional cubic cell. Derive analytical expressions for the structure factor,

$$S_G = \sum_j f_j e^{i\vec{G}\cdot\vec{r}_j},$$

for the monoatomic sc, fcc and diamond lattices. \vec{r}_j is the position of the j 'th atom in the (here) simple cubic unit cell, and f_j its atomic form factor. [6]

(c) Determine the reflections (hkl) that give rise to peaks in the diffraction pattern for sc and fcc, for all reflections up to (300), and show that two of the data columns are consistent with these. Hence identify all three structures. [6]

(d) Assuming that the lowest-order reflection for the diamond lattice is (111), find the length a of the conventional cubic cell side for all three samples. [5]

(e) Which general change would you see in the diffraction pattern for A, B, and C if f_j for the corner atoms in the conventional cubic cell were different from f_j for the other atoms? Explain your answer. [6]

10. The energy of a collection of oscillators of frequencies ω_K in thermal equilibrium is

$$U = \sum_K \underbrace{\frac{1}{\exp(\hbar\omega_K/k_B T) - 1}}_I \underbrace{\hbar\omega_K}_II,$$

where K is the wavenumber. For convenience, we have omitted the polarisation here.

(a) Describe the physical meaning of the terms I and II. [4]

(b) Assume a one-dimensional crystal of length L , consisting of N equidistant identical atoms. Use periodic boundary conditions to show that the density of K states is given by

$$D(K) = \frac{L}{2\pi}.$$

With this result, derive an integral expression for the energy U . [6]

(c) Which main two assumptions are made in the Debye theory? [6]

(d) Show that these assumptions lead to the following expression for U :

$$U = \frac{Lk_B^2 T^2}{2\pi v_s \hbar} \int_0^{x_D} \frac{x}{e^x - 1} dx.$$

The calculation of x_D is not requested here. [9]

(e) Some materials consist of weakly coupled, nearly one-dimensional structures, leading to material properties that strongly deviate from three-dimensional materials. Based on the result in (d) and on the low-temperature limit of the standard (three-dimensional) Debye model, suggest an experiment to determine whether a material is one- or three-dimensional. You may use the result

$$\int_0^\infty \frac{x}{e^x - 1} dx = \frac{\pi^2}{6}.$$

[5]