Answer any THREE questions.

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}
Permeability of free space	μ_0	$=$	$4\pi \times 10^{-7}$ H m^{-1}
Bohr magneton	μ_{B}	$=$	9.273×10^{-24} J T^{-1}
Boltzmann's constant	k_{B}	$=$	1.38×10^{-23} J K^{-1}
Planck's constant/2π	$\hbar$	$=$	1.05×10^{-34} J s

[Part marks]

1. (a) Explain the terms *lattice*, *basis* and *unit cell*. State the number of lattice points in the conventional cubic unit cell for the face-centred cubic lattice. **[4]**

   (b) The primitive translation vectors of the face-centred cubic lattice are those joining a lattice point at the origin to three of its nearest neighbours. Calculate the primitive vectors of the reciprocal lattice for this structure. **[5]**

   (c) Explain what is meant by *missing orders* in diffraction from crystals.

   If a cubic crystal with cubic cell side 0.42 nm is illuminated with X-rays of wavelength 0.154 nm, at what angles away from the incident beam will the five lowest-order diffracted beams be expected?

   Which of these beams will be observed if the crystal has a face-centred cubic structure? **[6]**

   (d) RbF forms face-centred cubic crystals, with a basis of Rb^+ at $(0,0,0)$, F^- at $(\frac{1}{2},0,0)$. How many nearest neighbours does each ion have, and how are they arranged?

   The cohesive energy per ion pair is written as

   $$U(r) = A\exp(-r/\rho) - \frac{\alpha q^2}{4\pi\epsilon_0 r},$$

   where r is the nearest-neighbour separation, q is the ionic charge, and $\alpha = 1.748$. Explain briefly the origin of the two terms in the energy. If $\rho = 0.03$ nm and the equilibrium value of the nearest-neighbour separation is 0.282 nm, what is the value of A? **[5]**

2. (a) Show that the density of states in each phonon mode in an isotropic three dimensional crystal is

$$g(\omega) = \frac{V}{2\pi^2} k^2 \frac{\mathrm{d}k}{\mathrm{d}\omega},$$

where ω is the phonon frequency, k is the phonon wavevector, and V is the volume of the crystal. **[5]**

(b) What are the assumptions of the Debye model for the specific heats of insulators? What is the significance of the Debye frequency ω_{D}? **[5]**

(c) The thermal energy of a three-dimensional crystal may be written as

$$U(T) = A \int_0^{\omega_D} \frac{\omega^3}{\exp(\hbar\omega/k_{\mathrm{B}}T) - 1} \mathrm{d}\omega,$$

where A is independent of temperature. Deduce the temperature dependence of the specific heat in the limits of low temperature and high temperature. **[5]**

(d) Two specimens of pure alumina, an electrical insulator, are obtained: one is a single crystal in the form of a cube of side length $1\ \mathrm{mm}$, and the other is a polycrystalline specimen in which the crystallites are $1\ \mu\mathrm{m}$ in size, and may be taken to be cubic in shape. Explain, with reasons, what you would expect to be the ratio of the thermal conductivities of the two specimens (i) at $4\ \mathrm{K}$; (ii) at $1000\ \mathrm{K}$. The Debye temperature of alumina is about $1000\ \mathrm{K}$. **[5]**

3. (a) What is meant by a degenerate Fermi gas? Briefly describe the following phenomena in simple metals: contact potential; thermal emission of electrons; and field emission. **[5]**

(b) The density of states in a free electron gas may be written as

$$g(E) = B\sqrt{E},$$

where B is a constant and E is the electronic kinetic energy. Show that the density of states at the Fermi surface may be written as

$$g(E_{\mathrm{F}}) = \frac{3N}{2E_{\mathrm{F}}},$$

where N is the total number of electrons in the sample.

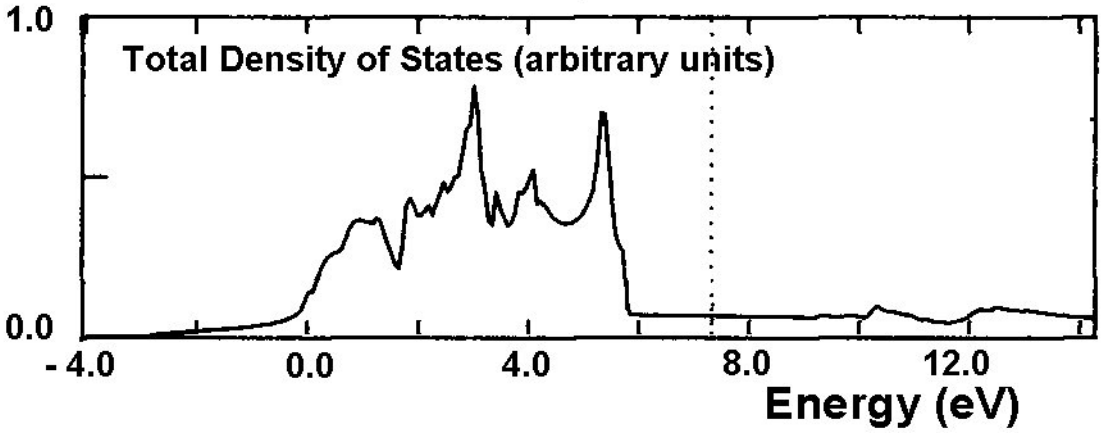
Given that for a sample of volume V

$$B = \frac{V}{2\pi^2}\left(\frac{2m_{\mathrm{e}}}{\hbar^2}\right)^{3/2},$$

calculate the Fermi energy of gold, treating gold as a free electron metal in which the electron concentration is $5.9 \times 10^{28}\ \mathrm{m}^{-3}$.

Use the expression for the density of states at the Fermi surface to estimate the size of a cube of gold for which the spacing of states at the Fermi surface is $\frac{1}{40}\ \mathrm{eV}$. **[9]**

(c) The graph below shows the calculated electronic density of states as a function of energy in gold. The dotted line marks the Fermi energy.



Comment on the general shape of the curve, including the underlying smooth curve and the structure between about $0\ \mathrm{eV}$ and $+6\ \mathrm{eV}$. Relate the curve to the colour of gold: note that the visible spectrum includes red light with an energy of about $1.5\ \mathrm{eV}$ and blue light at about $2.5\ \mathrm{eV}$ **[6]**

4. (a) In a tight binding model of the electronic structure of a one-dimensional solid, the matrix elements of the Hamiltonian H between atomic functions $\phi_j(r)$ centred on sites j satisfy

$$\begin{aligned}
\int \phi_i^*(r)\mathsf{H}\phi_i(r)\,\mathrm{d}r &= -\alpha \\
\int \phi_i^*(r)\mathsf{H}\phi_j(r)\,\mathrm{d}r &= -\beta \text{ if } i \text{ and } j \text{ are nearest neighbours,} \\
\int \phi_i^*(r)\mathsf{H}\phi_j(r)\,\mathrm{d}r &= 0 \text{ otherwise}
\end{aligned}$$

and also

$$\int \phi_i^*(r)\phi_j(r)\,\mathrm{d}r = \delta_{ij},$$

where the integrals are taken over the whole crystal and $\delta_{ij} = 1$ if $i = j$, 0 otherwise.

A wavefunction of the form

$$\psi_k(r) = \sqrt{\frac{1}{N}} \sum_{n=1}^{N} e^{ikna}\phi_n(r)$$

is assumed for a closed chain of N atoms spaced a apart with periodic boundary conditions in which atom 1 is joined to atom N. Show that this wavefunction is normalised, and evaluate its energy in terms of k, α and β. **[5]**

(b) Sketch the resulting dispersion relation for values of k between $-\pi/a$ and π/a. What is the width of the band formed by these states?

Calculate the effective mass of an electron near the bottom of this band, and for one near the top of the band. Hence, using the fact that the valence band in a semiconductor is usually narrower in energy than the conduction band, would you expect a hole in a semiconductor to be heavier or lighter than an electron? **[7]**

(c) An electric field $\mathcal{E}$ is applied to the system. Calculate the total current in the system when the band is filled. **[4]**

(d) Show, by imposing periodic boundary conditions on the chain, that for any two different allowed values of k and k' the states ψ_k and $\psi_{k'}$ are orthogonal. **[4]**

5. (a) Explain the origins of diamagnetism and of paramagnetism in insulating solids. Which of these behaviours is exhibited by a superconductor below its transition temperature? **[4]**

(b) Give a brief description of the phenomenon of *quenching* of orbital angular momentum in solids. Explain why quenching affects transition metals much more strongly than rare earths. **[6]**

(c) A salt of Vanadium containing V^{3+} ions has spin $S = 1$ and to a good approximation there is no contribution from the orbital angular momentum to the magnetic moment. Show that, if there are n ions per volume, the equilibrium magnetisation in a field $\mathcal{B}$ is

$$\mathcal{M} = 2n\mu_{\rm B}\frac{2\sinh(x)}{2\cosh(x)+1},$$

where $x = 2\mu_{\rm B}\mathcal{B}/(k_{\rm B}T)$. Sketch the form of the magnetisation as a function of $\mathcal{B}/T$.

Show also that in the limit of small $\mathcal{B}/T$ the susceptibility follows Curie's law, $\chi = C/T$, and give an expression for the constant C. Evaluate the low-field susceptibility at 300 K when there are 10^{27} ions per cubic metre. **[10]**

END OF PAPER