

**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	$m_e$	=	$9.11 \times 10^{-31}$ kg
Charge on the electron	$e$	=	$-1.602 \times 10^{-19}$ C
Permittivity of free space	$\epsilon_0$	=	$8.854 \times 10^{-12}$ F m <sup>-1</sup>
Boltzmann's constant	$k_B$	=	$1.38 \times 10^{-23}$ J K <sup>-1</sup>
Planck's constant/ $2\pi$	$\hbar$	=	$1.05 \times 10^{-34}$ J s
Speed of light	$c$	=	$3 \times 10^8$ m s <sup>-1</sup>

## SECTION A

[Part marks]

- Using the conventional unit cell draw cross-sections perpendicular to the [001] direction through the face centred cubic (*fcc*) structure for  $z=0$ ,  $a/2$  and  $a$ , where  $a$  is the cubic unit cell parameter. [3]

Calculate the maximum packing fraction of an ideal FCC solid. [4]

- For an ionic solid such as NaCl the cohesive energy per ion pair may be written as

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

where  $r$  is the nearest neighbour distance,  $Z$  is the ionic charge,  $\rho$  is a material dependent length scale, and  $\alpha=1.748$ .

Explain briefly the origins of the two terms. [2]

Show that  $A = \alpha Z^2 \rho \exp(r_0/\rho) / (4\pi\epsilon_0 r_0^2)$  where  $r_0$  is the equilibrium separation. [4]

- State Bragg's law for the constructive interference of X-rays of wavelength  $\lambda$  scattered through an angle  $2\theta$  by lattice planes of spacing  $d$  in a crystal. [2]

What is the relationship between the lattice plane spacing  $d$ , the lattice constant  $a$ , and the Miller indices  $(h, k, l)$  for a cubic system? [2]

Calculate the expected scattering angles  $2\theta$  of the three lowest order diffraction peaks from a simple cubic lattice of spacing  $a=0.335$  nm if  $\lambda=0.150$  nm. [3]

4. Explain why in a free electron metal it is not possible for all electrons to have the same energy. [2]

Provide definitions of the following: Fermi energy, Fermi temperature and Fermi surface. [3]

Why is the specific heat of simple metals at room temperature much lower than that calculated for a classical gas of electrons? [2]

5. The frequency  $\omega$  and wavenumber  $K$  of longitudinal phonons (lattice vibrations) propagating along a one dimensional chain of atoms are related to each other by the dispersion relation

$$\omega = \sqrt{\frac{4C}{M}} |\sin(Ka/2)|$$

where  $C$  is the force constant,  $a$  is the equilibrium spacing between the atoms and  $M$  is the atomic mass.

Make a sketch of the dispersion relation, being careful to label the axes appropriately. Identify the location of the Brillouin zone boundary. [2]

Derive an expression for the *group velocity* from the phonon dispersion relation. Give a physical explanation for the value of the phonon group velocity at the Brillouin zone boundary. [4]

6. Write down the expression for the kinetic energy  $E_k$  of a free electron of wavevector  $k$ , and show how the electron mass can be written in terms of a derivative of  $E_k$ . [3]

Make a sketch of a simplified  $E_k$  versus  $k$  relationship for an electron propagating in a direct bandgap semiconductor near the band edges. Indicate on the sketch the valence and conduction bands, and for these bands comment on whether the effective mass of the electrons is expected to be positive or negative. [4]

## SECTION B

7. State the key assumptions used in the Debye theory of the specific heat of insulating solids. [3]

Show that the phonon density of states as a function of frequency  $\omega$  in three dimensions is given in Debye theory by

$$g(\omega) = \frac{V}{2\pi^2} \frac{\omega^2}{v_s^3}$$

where  $V$  is the sample volume and  $v_s$  is the speed of sound. [6]

Explain why according to Debye theory the internal energy  $U$  of a solid may be written as

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

where  $A$  is a constant independent of temperature and  $\omega_D$  is the Debye frequency. (You do not need to explicitly evaluate  $A$  or  $\omega_D$ .) [7]

Derive an expression for  $U$  in the limit of low temperature, and hence determine the temperature dependence of the specific heat  $C_V$  in this limit. (Note:  $\int_0^\infty x^4 e^x / (e^x - 1)^2 dx = 4\pi^2/15$ .) [8]

Without recourse to detailed calculations determine the dependence of  $C_V$  on temperature in the low temperature limit for two and one dimensional insulators. [6]

8. Consider a two dimensional metal with a square lattice of spacing  $a$  for which the electrons may initially be considered to be free.

Write down a general expression for a reciprocal lattice vector of the two dimensional square lattice in terms of  $a$ . Draw a sketch of the reciprocal lattice close to the origin, and identify the area of the first Brillouin zone. [6]

By evaluating the ratio of the area of the first Brillouin zone to the density of states as a function of wavevector  $\mathbf{k}$ , show that the first Brillouin zone contains exactly  $2N$  electron states, where  $N$  is the number of atoms. [6]

In the case that the metal is monovalent, calculate the magnitude of the Fermi wavevector  $k_F$ , and make a sketch of the Fermi surface in reciprocal space being sure to indicate the position of the boundaries to the first Brillouin zone. Indicate on a separate sketch the displacement of the Fermi surface produced by an electric field along the  $x$  direction. [9]

It is now assumed that the metal is divalent, and that the electrons are affected by the periodic potential of the ion cores. Discuss with the aid of sketches how the shape of the Fermi surface evolves as the strength of the periodic potential is increased. [9]

9. This question is about X-ray scattering from chromium which crystallises in the body centred cubic (*bcc*) structure.

Using the conventional cubic cell identify the lattice and the basis needed to generate the *bcc* structure, and hence derive the unit cell structure factor, being careful to define any terms that you introduce.

[6]

What is the condition on the Miller indices ( $h, k, l$ ) for the Bragg reflections to have non-zero intensity?

[4]

A diffraction experiment is performed on chromium using radiation with a wavelength of  $\lambda=0.100$  nm. The first three Bragg reflections are recorded at scattering angles  $2\theta$  of 28.43, 40.64, 50.33 degrees. Using this data assign Miller indices to these reflections and deduce the lattice parameter  $a$  of chromium.

[12]

In terms of the conventional cell, the reciprocal lattice vectors can be written in Cartesian coordinates as  $\mathbf{G} = (2\pi/a)(h, k, l)$ . Draw sections of reciprocal space for  $l = 0, 1$ , and  $2$  with  $h$  and  $k$  restricted to the range  $-1 \leq h, k \leq 1$ , and for each section indicate by a filled circle the locations of the allowed Bragg peaks for the *bcc* structure. Use this information to deduce the reciprocal lattice of the *bcc* lattice. How else might you have arrived at the same conclusion by direct calculation? Be sure to state the relevant formulae required, although it is not necessary to evaluate them for the specific case of *bcc*.

[8]

10. With the aid of energy versus wavevector diagrams explain what is meant by the terms *intrinsic* and *extrinsic* semiconductors. Indicate on your diagrams the states that can give rise to extrinsic behaviour and explain how they are typically introduced, taking care to define any terms you use. [6]

The density of electron states  $g(\mathcal{E})$  in the conduction band of a semiconductor with an energy gap  $\mathcal{E}_G$  is given by

$$g(\mathcal{E}) = \frac{V}{2\pi^2\hbar^3} (2m_e^*)^{3/2} (\mathcal{E} - \mathcal{E}_G)^{1/2}$$

where  $m_e^*$  is the effective mass of the electron,  $V$  is the volume and the zero of energy is equal to the top of the valence band. Show that the number of electrons per unit volume in the conduction band is given by

$$n = N_C e^{(\mu - \mathcal{E}_G)/k_B T}$$

where  $N_C$  is a temperature dependent constant and  $\mu$  is the chemical potential. (Note:  $\int_0^\infty x^{1/2} e^{-x} dx = \sqrt{\pi}/2$ .) [8]

Derive the corresponding expression for the number of holes  $p$  per unit volume in the valence band and hence derive the law of mass action

$$np = N_C N_V e^{-\mathcal{E}_G/k_B T}$$

where  $N_V$  is another temperature dependent constant. [8]

Consider a sample of silicon ( $\mathcal{E}_G=1.1$  eV) which has been purified until it contains only  $10^{18}$  impurities  $\text{m}^{-3}$ . The intrinsic carrier concentration of silicon at 300 K is  $2 \times 10^{16} \text{m}^{-3}$ . Show that the temperature  $T_i$  above which silicon exhibits intrinsic behaviour can be written as

$$8.8 \approx \frac{6380}{T_i} - \frac{3}{2} \log_e T_i$$

and hence estimate  $T_i$ . [8]