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

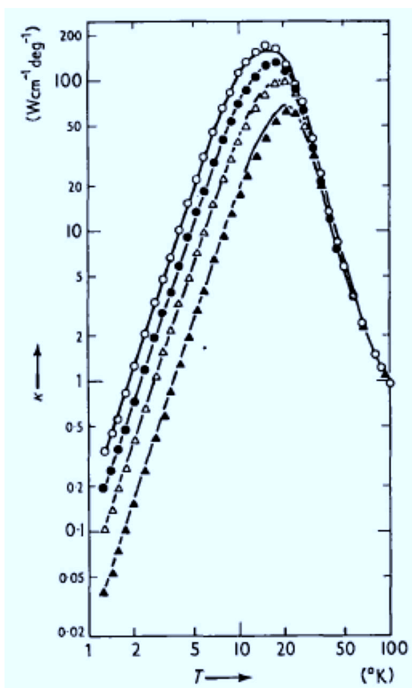
The numbers in square brackets in the right-hand margin indicate the provisional allocation of maximum marks per sub-section of a question.

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
Speed of light	c	$=$	3×10^8 m s^{-1}

SECTION A **[Part marks]**

1. Sketch how a crystal lattice becomes distorted in the presence of an *edge dislocation*. **[3]**

   Describe how the strength of materials can be reduced by the presence of dislocations. **[3]**



2. The graph above shows the thermal conductivity of several samples of LiF measured as a function of temperature. What physical process is responsible for the conductivity increasing with temperature on the left side of the graph? **[3]**

   What physical process is responsible for the conductivity decreasing with temperature on the right side of the graph? **[3]**

3. Sketch the dispersion relation of the mechanical waves travelling in a one-dimensional crystal made of alternating atoms of different masses, connected with identical springs. Label the axes. Label the various branches with their usual names. **[3]**

   Describe all the possible motions of the atoms in the allowed (longitudinal) waves in the long wavelength limit. **[4]**

4. An Aluminium ($Z = 13$) atom substitutes for one of the silicon ($Z = 14$) atoms in a crystalline block of silicon. Explain how its bonding into the lattice gives rise to a 'hole'. **[4]**

   Show with the aid of a suitable diagram where the energy of this 'hole' lies with respect to the electronic levels of the silicon host. **[3]**

5. A hypothetical potential function is proposed for the interaction between two atoms of an inert gas,

$$U(r) = U_0 \left[\left(\frac{r_0}{r} \right)^9 - \left(\frac{r_0}{r} \right)^6 \right]$$

   Which of the two terms represents the *attractive* part of the potential? **[3]**

   A molecule is composed of three atoms of the gas in a triangular configuration. What is its equilibrium bond length? **[4]**

6. What are the allowed energies of free electrons occupying a one-dimensional box of length L? Sketch some typical wave functions. **[4]**

   If N electrons are placed in the box in the minimum energy configuration (at $T = 0$), what is the energy of the most energetic electron? **[3]**

SECTION B

7. A *monovalent* element forms a two-dimensional solid with a rectangular unit cell of lattice constants a and b with $a > b$ and one atom per unit cell. Consider the allowed states of *free* electrons in a finite piece of the substance with dimensions $L \times L$.

   (a) Is it generally expected that a monovalent solid would be a metal or an insulator? Why so? **[5]**

   (b) Draw labelled diagrams of the direct space lattice and the corresponding reciprocal lattice showing the first Brillouin Zone and the free-electron Fermi surface. Indicate clearly which states are filled and which are empty at $T = 0$. **[7]**

   (c) What condition(s) on a and b are required for the free electron Fermi surface to extend into the second Brillouin Zone? Illustrate how this transition takes place in your reciprocal space diagram of the material. **[8]**

   (d) Now consider the nearly-free electron approximation where a band gap opens at the zone boundary. Show how the Fermi surface distorts instead of filling the second zone. **[4]**

   (e) If you could continuously distort the lattice through this transition, how would you expect the electrical conductivity to vary along the a and b directions? **[6]**

8. In two dimensions, the Debye theory of the specific heat of a solid predicts the internal energy of a solid containing N atoms to be:

$$U = X(T) \int_0^{x_D} \frac{x^2 dx}{e^x - 1}$$

   where $x = \hbar\omega/k_B T$ is the dimensionless form of the vibration frequency. In this problem, you may find it helpful to use the symbol ζ_2 for following standard definite integral $\zeta_2 = \int_0^\infty \frac{x^2 dx}{e^x - 1}$.

   (a) According to this theory, what is the physical origin of the internal energy? What are the standard approximations made in the Debye model? **[8]**

   (b) Derive an expression for the quantity x_D which appears above in terms of these approximations. **[6]**

   (c) By equating the *high-temperature* limit of the above expression to the classical 2D result $U = 2Nk_BT$, deduce the unknown function $X(T)$. **[7]**

   (d) Hence derive an expression for the *low-temperature* specific heat of a 2D solid in the Debye theory. **[9]**

9. (a) Sketch the typical energy band diagram for electrons in a semiconductor, indicating which states are empty and which are filled at $T = 0$. Which part(s) of the diagram are responsible for the "effective masses" m_e^* and m_h^*? Label the energies of the conduction and valence band edges as E_C and E_V. **[8]**

(b) Deduce an expression for the "density of states", the number of electron states per unit energy in the conduction band in terms of E_C and m_e^*. **[6]**

(c) Hence derive the following expression for the total number of electrons per unit volume in the conduction band,

$$n = 2\left(\frac{m_e^* k_B T}{2\pi\hbar^2}\right)^{3/2} e^{(\mu - E_C)/k_B T}.$$

You may wish to use the standard integral $\int_0^\infty \sqrt{x} e^{-x} dx = \frac{1}{2}\sqrt{\pi}$. **[9]**

(d) What physical significance it attributed to the symbol μ? By equating the expression above with an equivalent one for the number of holes in the valence band, deduce an equation for μ for an intrinsic semiconductor. **[7]**

10. The diffraction angles of the first three peaks of the powder diffraction pattern, measured from a certain sample at room temperature, are listed below. X-rays of wavelength $\lambda = 0.1542nm$ were used.

When the sample is cooled, some of the peaks are found to split into pairs of two angles given in the second column.

2θ angle Room temperature	2θ angle Low temperature	
$22.80°$	$22.69°$	$22.86°$
$32.47°$	$32.43°$	$32.55°$
$40.05°$	$40.05°$	

(a) Why is diffraction only seen at these angles shown and not in between? State the law that connects the Bragg angle, θ, and the crystal lattice spacing. **[6]**

(b) Deduce the crystal symmetry and the lattice parameter of the room temperature sample from the observed angles. **[10]**

(c) At what 2θ angle would you expect the next peak to appear for the room temperature sample? **[6]**

(d) Explain with as much detail as possible what happens to the crystal structure at low temperature. **[8]**