



Answer only and only 5 questions: (Each question = 16 Marks)

1. :

- a. Describe how the solids structures, e.g., a crystal of NaCl is more stable than a collection of free Na and Cl atoms?
- b. In short notes, write the main types of bonding in solids?

2. : a)

- i. Crystal lattice: one replaces each atom by a geometrical point located at the equilibrium position of that atom. Simply, all the atomic sites have been replaced by lattice sites.
 - ii. pravais and non-pravais lattice: In a Bravais Lattice, all lattice points are equivalent, and hence by necessity all atoms in the crystal are of the same kind. On the other hand, in a non-Bravais lattice, some of the lattice points are nonequivalent.
- b. BCC $a = 4r/\sqrt{3} = 2.905 \text{ \AA}$ and volume $= a^3 = 24.251 \times 10^{-30} \text{ m}^3$
 Volume of each atom $= V_1$ of unit cell/no. atoms per unit cell $= 12.26 \times 10^{-30} \text{ m}^3$ and
 In FCC $a = 2\sqrt{2} r = 3.654 \text{ \AA}$ and $V_1(\text{unit cell}) = 48.787 \times 10^{-30} \text{ m}^3$
 No. atoms per unit cell = 4
 Volume of each atom = v. of unit cell of FCC/no. of atoms per unit cell $= 12.2 \times 10^{-30} \text{ m}^3$
 The % volume change $= (V_1 - V_2/V_1) \times 100 = 0.5\%$

3. :

- a. How X-ray is produced? And why we X-ray is used in crystallography?
- b. Electrons are accelerated by 8.54 kV and are reflected by a crystal. The first reflection maximum occurs when the glancing angle is 56° . Estimate the spacing of the crystal.

4. :

- a. According to the classical free electron theory, calculate the resistivity of metal and describe the electrical resistivity versus temperature.

$$m_e \left(\frac{d\vec{v}}{dt} + \frac{\vec{v}}{\tau} \right) = -e\vec{E} - e\vec{v} \times \vec{B} \quad \text{And} \quad \vec{v} = -\frac{e\tau}{m_e} \vec{E} \quad \mu_e = \frac{e\tau}{m_e}$$

$$\boxed{J = n(-e)v} \quad n = \frac{N}{V}$$

$$\vec{J} = \frac{ne^2\tau}{m_e} \vec{E} \quad \sigma = \frac{ne^2\tau}{m_e}$$

$$\boxed{\vec{J} = \sigma \vec{E}} \quad \rho = \frac{1}{\sigma} \quad R = \frac{\rho L}{A}$$

- b. Explain the assumptions to overcome the drawbacks of the electrical resistivity versus temperature.



In a perfect crystal; the collisions of electrons are with thermally excited lattice vibrations (scattering of an electron by a phonon). This electron-phonon scattering gives a temperature dependent collision time which tends to infinity as $T \rightarrow 0$. In real metal, the electrons also collide with impurity atoms, vacancies and other imperfections, this result in a finite scattering time even at $T=0$.

The total scattering rate for a slightly imperfect crystal at finite temperature;

$$\frac{1}{\tau} = \frac{1}{\tau_{ph}(T)} + \frac{1}{\tau_0}$$

So the total resistivity ρ ,

$$\rho = \frac{m_e}{ne^2\tau} = \frac{m_e}{ne^2\tau_{ph}(T)} + \frac{m_e}{ne^2\tau_0} = \rho_l(T) + \rho_0$$

This is known as Mattheisen's rule and illustrated in following figure for sodium specimen of different purity.

5. :

a. When can be treated a crystal as a continuous medium?

In the long-wavelength limit, a crystal may be treated as a continuous medium because the wavelength is much greater than the lattice constant.

b. Define Dulong-Petit law and explain how Einstein rectified the discrepancy when applying this law?

The atoms in the lattice are regarded as a set of harmonic oscillators, and the thermal energy is the average energy of these oscillations. According to classical theory, the average energy for a one-dimensional oscillator is

$$\bar{E} = kT$$

Thus the total thermal energy per mole is $\bar{E} = 3 N_A kT$ and $C_v = \frac{\partial \bar{E}}{\partial T} = 3R$

where $R = N_A k$ is the universal gas constant. This result, known as the Dulong-Petit law, asserts that C_v is a constant independent of temperature. This law is found to be valid only at high temperatures; at low temperatures, specific heat decreases and then vanishes at $T = 0K$.

Einstein rectified this discrepancy by treating the oscillator quantum mechanically. The average thermal energy for the oscillator is then given by

$$\bar{E} = \frac{\hbar\omega}{e^{\hbar\omega/kT} - 1}$$

Treating the atoms as independent oscillators, vibrating with a common frequency, Einstein found that the specific heat is

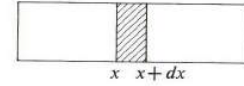
$$C_v = \frac{\partial \bar{E}}{\partial T} = 3R \left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E}}{(e^{\theta_E} - 1)^2}$$

where θ_E is the Einstein temperature



6. What is the concept of term density of states and derive it?

The density of states $g(\omega)$ is defined, as before, such that $g(\omega) d\omega$ gives the number of modes in the frequency range $(\omega, \omega + d\omega)$. This function plays an important role in most phenomena involving lattice vibrations, particularly specific heat.



Consider first the one-dimensional case.

Consider the elastic waves in the long bar of Fig., in which the wave travels in one dimension only. The solution has already been written in (3.5). That is,

$$u = Ae^{iqx} \quad (1)$$

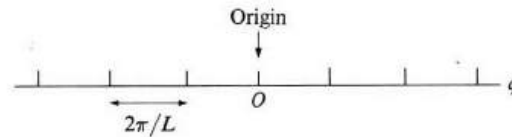
It is as if the bar were deformed into a circular shape so that the right end joined the left. Given that the length of the bar is L , if we take the origin as being at the left end, the periodic condition means that

$$u(x=0) = u(x=L), \quad (2)$$

where u is the solution given in (1). If we substitute (1) into (2), we find that $e^{iqL} = 1$ (3)

This equation imposes a condition on the admissible values of q ; only those values which satisfy (3) are allowed. Noting that $e^{in2\pi} = 1$ for any integer n , we conclude from (3) that the allowed values are $q = n \frac{2\pi}{L}$ (4) where $n = 0, \pm 1, \pm 2, \dots$

When these values are plotted along a q -axis, they form a one-dimensional mesh of regularly spaced points, as shown in Fig (2). The spacing between the points is $2\pi/L$. When the bar length is large, the spacing becomes small and the points form a quasi-continuous mesh. Each q -value of (4), or each point in Fig.2, represents a mode of vibration. Suppose we choose an arbitrary interval dq in q -space, and look for the number of modes whose q 's lie in this interval. We assume here that L is large, so that the points are quasi-continuous; this is true, of course, for the macroscopic objects with which we are dealing. Since the spacing between the points is $2\pi/L$, the number of modes is $(L/2\pi)dq$ (5)



But q and the frequency ω are interrelated via the dispersion relation, and we may well seek the number of modes in the frequency range $d\omega$ lying between $(\omega, \omega + d\omega)$. The density of states $g(\omega)$ is defined such that $g(\omega)d\omega$ gives this number.

$$g(\omega) = \frac{L}{\pi} \frac{1}{d\omega/dq}$$

With my best wishes &