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Out lines :-

- ♦ Classical Theory for specific heat
- ♦ Einstein Theory for specific heat
- ♦ Thermal expansion

Introduction :-

● Thermal properties of solids depend on the vibration of the atoms, that is, on the lattice motion.

● Heating a solid means giving the atoms extra energy that enables them to vibrate around their equilibrium positions.

● The physical concept of heat is the transfer of energy, where the energy is transferred from one location to another by means of phonons, which is defined as the amount of energy of vibration of the lattice.

● The heat capacity (C) of the solids of a system is the amount of heat needed to raise the temperature of that system by one degree.

● Specific heat is the amount of heat required to raise the temperature of one gram of a substance by one degree, and is given by the following relationship: $C = Q / T$.

Note that the capacitance changes with temperature.

Theoretical models to explain the change in heat capacity with temperature :-

1. Classical Theory for specific heat :-

As we explained earlier that a solid is made up of atoms bonded to each other by a harmonic force. For the purpose of clarifying the theory, we suppose that an atom of mass m in a crystal moves in a simple harmonic motion with amplitude (A) and angular frequency (w) under the influence of a linear return force. If we consider that the displacement of the atom at any moment from the position of equilibrium is (x), then its velocity is (v) and its acceleration is a, and the total energy accompanying the oscillating atom is E :-

$$E = T + V = \frac{1}{2}\, m\, v^2 + \frac{1}{2}\, m\, x^2$$

$$= \frac{1}{2}\,(m\, v^2 + m\, x^2)$$

And by applying classical statistical mechanics to obtain the expected value of the energy E for a single oscillating atom :

$$\langle E \rangle = \frac{\int_0^{V_m}\int_0^{x_m} E \exp\left(-E/K_B T\right) dx\, dv}{\int_0^{V_m}\int_0^{x_m} \exp\left(-E/K_B T\right) dx\, dV} = K_B T$$

The vibrational energy (U) of a crystal containing N atoms :-

$$U = 3\,N\,K_B T$$

Therefore, the specific heat at a constant volume is :-

$$C_V = \left(\frac{dU}{dT}\right)_V = 3NK_B$$

Since the general constant for gases is :

$$R = N\,K_B = 8.3142\ \ J/\,mol.\,k$$

$$C_V = 3\,R = 25\ J/\,mol.\,k$$

It is clear from the above equation that specific heat does not depend on temperature in the classical theory.

2. Einstein Theory for specific heat :-

● In this model, Einstein assumed that the atom vibrates independently (that is, each atom is considered a simple harmonic oscillation independent of the other oscillations), so that the crystal can be considered as having (N) harmonic oscillations with an angular frequency (w).

● Einstein adopted the average energy of an oscillator according to Planck's theory, which states that any oscillator emits or absorbs energy (hv) multiplied by an integer n.

$$E_n = nhv$$

● The total vibrational energy of the crystal is given by the following relationship :

$$U = \frac{3N\hbar w}{e^{\frac{\hbar w}{K_B T}} - 1}$$

Therefore, the specific heat capacity is given by the following relationship :

$$C_V = 3R\left(\frac{\hbar w}{K_B T}\right)^2 \frac{e^{\frac{\hbar w}{K_B T}}}{\left(e^{\frac{\hbar w}{K_B T}} - 1\right)^2}$$

$$\mathbf{C_V = 3R\ F_E(W_E, T)}$$

Where F_E (W_E, T) : is the Einstein function.

We conclude from the above the following :

1. At higher temperatures, the Einstein function becomes : $F_E(W_E, T) = 1$

So, the value of heat capacity is : $C_V = 3\ R$

2. At low temperatures, the Einstein function becomes:

$$F_E(W_E, T) = (T_E/T)^2 \exp(-T_E/T)$$

So, the value of heat capacity is: $C_V = 3R(T_E/T)^2 \exp(-T_E/T)$

Thermal Expansion :-

♦ A change in the temperature of a substance leads to changes in other properties of the substance, and one of these changes is a change in the dimensions of the substance or a change in its state.

♦ Increasing the temperature of the material leads to an increase in the vibrational energy, and when the amplitude of vibration of these particles increases, the dimensions of the material will change.

♦ Most objects expand when their temperature increases, and the amount of material expansion depends on the amount of cohesive forces between its molecules.

♦ The amount of expansion of a solid by heating is very small due to the large cohesive forces between its molecules.

♦ This phenomenon plays a major role in many engineering applications, for example, spaces are left between the steel joints in buildings to give room for expansion and contraction.

♦ We conclude from this that thermal expansion is the result of the change that occurs in the distances between molecules and atoms of a substance.

♦ In the expansion of solid bodies, the expansion occurs over the entire body, such as length, width, and thickness, and the increase in length is more than in width or thickness.

♦ Experiments have proven that the change in length is directly proportional to the change in temperature and the original length, so the equation for the change in length can be written as follows:-

$$\Delta L = \alpha L \Delta T$$

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