ASSIGNMENT
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Anharmonic Effect In Crystals

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Submitted By:

Aman Tiwari

Class :-

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Roll No. :- 191022683

School of Studies in Physics

Jiwaji UNIVERSITY, GWALIOR.

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Anharmonic Effect In Crystals

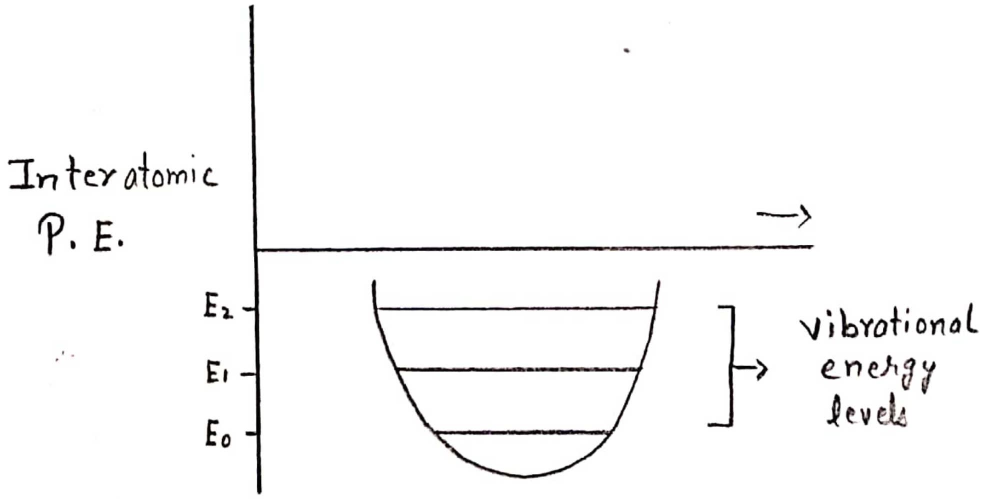
For harmonic approximation, the elastic force acting on a particle displaced from their equilibrium position is proportional to the displacement and is directed towards the equilibrium position.

$$f = -\beta x \qquad \{ \beta \text{ is elastic constant}$$

and the corresponding potential energy is

$$U(x) = -\beta \frac{x^2}{2}$$

The graphical representation of this equation is



Indicating that, amplitude of the atomic lattice vibrations increase with the increase in temperature.

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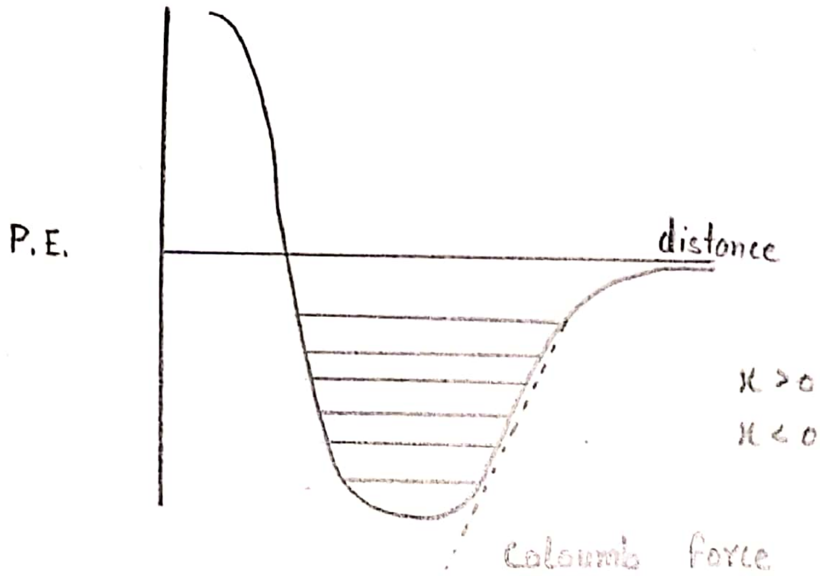
As the temperature increases, the solid expands implying that the vibrations of the particles in solid are not truely harmonic i.e. their occurs ~~ah~~ anharminicity in the solid.



$$U(x) = \beta \frac{x^2}{2} - g \frac{x^3}{3}$$

$$f(x) = -\frac{\partial U}{\partial x} = -\beta x + g x^2$$

Now we define average interatomic spacing i.e. $\bar{x}$. The value of thermal expansion coefficient

$$\bar{f} = -\beta \bar{x} + g \bar{x}^2$$

However, when the particle vibrate freely i.e. $\bar{f} = 0$

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$$\therefore \quad g\bar{x}^2 = \beta x$$

$$\Rightarrow \quad \bar{x} = g \cdot \frac{\bar{x}^2}{\beta}$$

For overoge potential energy of the vibrating particle can be written as

$$\bar{U}(x) \sim \beta \frac{\bar{x}^2}{2}$$

$$\bar{x}^2 \simeq 2 \frac{\bar{U}(x)}{\beta}$$

$$\therefore \quad \bar{x} = \frac{2g\,\overline{U(x)}}{\beta^2}$$

However in addition to the potential energy, the vibrating particle has Kinetic energy also such that,

$$\overline{U(x)} = E_K$$

$$\therefore \quad \text{Total energy} \quad \bar{E} = \bar{E}_K + \bar{U}(x)$$

$$\therefore \quad \bar{x} = g \frac{\bar{E}}{\beta^2}$$

The relative linear expansion is defined as the ratio of average interatomic spacing $(\bar{x})$ to the equilibrium interatomic spacing (r_0)

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is equal to

$$\frac{\bar{x}}{r_0} = \frac{g\bar{E}}{\beta^2 r_0}$$

and the coefficient of linear thermal expansion is given by

$$\alpha = \frac{1}{r_0}\frac{d\bar{x}}{dT}$$

$$\alpha = \frac{g}{\beta^2 r_0}\frac{d\bar{E}}{dT}$$

$$\boxed{\alpha = \chi C_v}$$

$\left\{ \text{where } \chi = \frac{g}{\beta^2 r_0} \right.$

where C_v is the specific heat of the solid of particle.

$$\boxed{\alpha_L = \frac{\gamma C_v K}{3V}}$$

where, α_L is the coefficient of linear expansion.
C_v is the molar specific heat
K is compressibility.
γ is the Gruneisens Parameter.
V is the molar volume.

where,

$$\gamma = -\frac{\ln \nu}{\ln V_a}$$

$\{$ ν is the frequency of atomic vibration and V_a is the atomic volume.

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