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A Classical Model for Study of Solids with Atom as Linear Oscillator

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Abstract: The purpose of present study was to apply a classical model for solid study. In the proposed model atoms were considered as points of mass having small oscillations near their equilibrium positions. Based on this consideration, the partition function was solved and with regard to equipartition theorem, its simplified equation has also been achieved. The model was applied to solid and necessary work for compressing solid, in order to obtain the compressibility factor as a function of solid volume and the temperature, has been calculated. A literal expression for pressure applied to solid and also an expression showing the compressibility variation have been deduced. For numerical application, aluminum was chosen as a solid in order to find out its parameters. The model can also easily be applied to other metals.

Key words: Classical approach, atom linear oscillation, work, compressibility factor, solid

INTRODUCTION

A low compressible solid of volume V, containing N atoms, assimilable to 3N identical, independent and linear oscillators at thermal equilibrium at T°, has been considered. The results of the linear oscillation modeling in conjunction with the approximation given by the energy equipartition theorem were successfully accepted. Each atom, being at rest and in its equilibrium, was considered to have a negative energy of $-E_0$, it has also been supposed that the initial position and energy; X_0 and E_0, were function of the volume V of solid.

At 0°K, the solid was considered as to be at equilibrium and at zero absolute pressure that is defined by V_0. The necessary work due to variation of compression from 0°K to any pressure P and at any temperature T, has been calculated with the help of Taylor series. The pressure P could be expressed as a function of solid volume V and of compressibility coefficient χ_0. The work resulted by the solid in compression phase from V_0 to V, has been deduced as a function of compressibility coefficient χ_0. The variation of compressibility as a function of temperature near equilibrium, which is defined by volume V_0, is also shown. This study has finally been applied to aluminum as an example of application but can easily be applied to other metals.

Modeling: An atom was considered as a point of mass m_0 and subjected to move along X-axis. Its energy can be given by[1];

$$U(X) = E_0 [(1\text{-Exp-}X_0X)^2\text{-}1)] \tag{1}$$

E_0 and X_0 having positive constant values. This atom can vibrate around its equilibrium position, which can be considered as a linear oscillator. The oscillation is due to thermal agitation resulted by temperature, T. It was supposed that $1/\beta = KT << E_0$, which implies that the atom vibrates at definite distance.

The atom is at its stable equilibrium when its potential energy is minimum, that means;

$$\partial U/\partial X = 2E_0X_0 (\text{Exp-}X_0X)(1\text{-Exp-}X_0X) = 0 \tag{2}$$

Hence, X=0.

Further we can have;

$$\partial^2U/\partial X^2|X_0 = 2E_0X^2_0 (\text{Exp-} X_0X) (2\text{Exp-}X_0X - 1)|_{X=0} = 2E_0X^2{}_0 > 0 \tag{3}$$

It is obvious that X=0 is a stable equilibrium position for the atom in question. As the system is a stationary system and not a relativistic one therefore, the Hamiltonian can be written as;

$$H_0 = T+U_0 \tag{4}$$

The oscillation energy at rest is zero therefore;

$$H_0 = P^2x /2m_0 + E_0(1\text{-Exp-}XX_0) \tag{5}$$

The partition function is then;

$$Z_C = \int_{-\infty}^{\infty} \text{Exp-}(P^2x\, \beta /2m_0)\, dPx \int_{-\infty}^{\infty} \text{Exp}[- \beta E_o(1\text{-Exp-}XX_0)^2]\, dX \tag{6}$$

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The dependence of X and t, can be written as[2];

$$t = 1 - \mathrm{Exp}\text{-}(XX_0) \quad (7)$$

$$dt = X_0\ \mathrm{Exp}\text{-}XX_0\ .\ dX = X_0(1\text{-}t)\ dX \quad (8)$$

Taking (8) into account, (6) will become;

$$Z_C = (1/X_0)\int_{-\infty}^{\infty} \mathrm{Exp}\text{-}(\ P^2x\ \beta\ /2m_0\ )\ dPx \int_{-\infty}^{1} (\mathrm{Exp}\text{-}(\beta E_0\ t^2)/(1\text{-}t\ ).dt \quad (9)$$

The left integration yields

$$Z_C = (1/X_0).\ (2\pi m_0\ /\beta)^{1/2}.\ \int_{-\infty}^{1}(\mathrm{Exp}\text{-}(\beta E_0\ t^2)/(1\text{-}t\ ).dt \quad (10)$$

For the second part integration, which is now based on time, one should go through following procedure;
We put;

$$I = \int_{-\infty}^{1} (\mathrm{Exp}\text{-}(\beta E_0\ t^2)/(1\text{-}t\ ).dt \quad (11)$$

We also put;

$$I_0 = \int_{-\infty}^{-1} (\mathrm{Exp}\text{-}(\beta E_0\ t^2)/(1\text{-}t\ ).dt \quad (12)$$

In addition we know that;

$$|I_0| \leq \int_1^{\infty} \mathrm{Exp}\text{-}(\beta E_0\ V^2)/(1\text{-}t).dt < \mathrm{Exp}\text{-}(\beta E_0 V^2).dv \ \fint_0^{\infty} (1/2).(\Pi/\beta E_0\ )^{1/2} \quad (13)$$

On the other hand we can have;

$$I_1 = \int_{-1+\epsilon}^{1-\epsilon} \mathrm{Exp}\text{-}(\beta E_0\ t^2)/(1\text{-}t).dt = \int_{-1+\epsilon}^{1-\epsilon}\mathrm{Exp}\text{-}(\beta E_0 t^2) \quad \sum_{n=0}^{\infty} t^n.dt \quad (14)$$

The convergence is uniform, therefore;

$$I_1 = \sum_{n=0}^{\infty} \int_{-1+\epsilon}^{1-\epsilon} t^n\,\mathrm{Exp}\text{-}(\beta E o t^2).dt \quad (15)$$

With the same procedure the second part integral will become as following;

$$I_1 = \sum_{p=0}^{\infty} \int_{-1}^{1} t^{2p}\,\mathrm{Exp}\text{-}(\beta E o t^2).dt \quad (16)$$

We can then have the following successive integrals;

$$I'_0 = \int_{-\infty}^{-1} t^{2p}\ \mathrm{Exp}\text{-}(\beta E_0 t^2).dt = \int_0^{\infty} t^{2p}\ \mathrm{Exp}\text{-}(\beta E_0 t^2).dt = I''_0 \quad (17)$$

$$|I'_0| = |I''_0| < \int_0^{\infty} t^{2p}\ \mathrm{Exp}\text{-}(\ \beta E_0 t^2).dt = I_{2p} \quad (18)$$

$$I_{2p} = \int_0^{\infty} t^{2p}\ \mathrm{Exp}\text{-}(\ \beta E_0 t^2).dt = (2\beta E_0)/(2p+1).I_{2P+2} =$$

$$1/2\sqrt{\pi/\beta E_0}.1/(2\beta E_0)^p \times 1 \times 2 \times 3 \times \ldots\ldots \times (2p-1) \quad (19)$$

On the other hand we can have;

$$\sum_{p=0}^{\infty} I_{2p} = \sqrt{\pi/\beta E_0}.\ \sum_{p=0} \frac{1*2*3\ldots.(2p-1)}{(2\beta E_0)^p} \quad (20)$$

The convergence factor Zc, can be written as following;

$$Zc = (1/x^2)\sqrt{\frac{2\pi m_0}{\beta}} \sum_{n=0}^{\infty} \int_{\infty}^{\infty} t^n\,\mathrm{Exp} - \beta E_0 t^n\ dt \quad (21)$$

Calculating (21),[2] yields;

$$Zc = (\pi/X_0\beta)\sqrt{2m_0/E_0}\ [1 + KT/(2E_0) + 0(\epsilon^2)] \quad (22)$$

Now the mean energy is;

$$u = \langle H_0 \rangle H_0 = KT^2 \frac{\partial}{\partial T}(\mathrm{Log}\ Zc) \quad (23)$$

As $KT/(2E_0) << 1$, then

$$U = KT\ [1 + KT/(2E_0)] \quad (24)$$

The proposed model yields a specific heat per atom gram greater than $3R_0$. The equipartition theorem attribute to a degree of free oscillation corresponding with energy of u=KT. In this case the simplified expression for Zc is presented as;

$$Zc = (\pi/X_0\beta)\sqrt{2m_0/E_0} \quad (25)$$

We are then guided to study the model for t tending to zero, which means for X tending to zero, therefore;

$$U(X) \approx E_0 X_0^2 X^2 \quad (26)$$

Hence;

$$F(X)\ \partial U/\partial X \quad E_0 X_0^2 X \quad (27)$$

This approximation shows that we are studying small movements of atom around equilibrium position of a quadratic potential.

Application to solid: In order to compose a solid a certain amount of work should be provided. This amount of work is then considered as internal energy of solid. The work provided is;

$$\tau' = -NE_0\ (V) \tag{28}$$

Each atom, at its equilibrium position, has a negative energy of - $E_0(V)$.
The internal energy of the solid can be written as;

$$U=+\tau=-\tau' =NE_0(V) \tag{29}$$

At zero Kelvin, the system can be considered at its equilibrium if its internal energy is minimal. By applying Taylor series we are able to deduce the necessary work for compressing the solid, at zero Kelvin and at zero pressure to a pressure of p, that is to say from volume V_0 to volume V;

$$E_0(V) = E_0(V_0)+(V-V_0)\ \frac{dE_0}{dV}|_{V_0} + \frac{(V-V_0)^2}{2}\ \frac{d^2E_0}{dV^2}|_{V_0}+\dots \tag{30}$$

Then;

$$\Delta\tau'=N\ \frac{(V-V_0)^2}{2}\ \frac{d^2E}{dV^2}|_{V_0} \tag{31}$$

The compressibility factor can be defined as;

$$\chi_0 = -\frac{1}{V_0}\ (\partial V/\partial P)_{T=0} \tag{32}$$

Calculating for dP, we can have;

$$dP = P = -\frac{1}{\chi_0 V_0}\ (V-V_0) \tag{33}$$

On the other hand we can have;s

$$\Delta\tau' = \int_{V_0}^{V} P\,dv = \frac{1}{\chi_0 V_0}\ \frac{(V-V_0)^2}{2} \tag{34}$$

Comparing (31) with (34), we can deduce for compressibility factor as;

$$1/\chi_0 = -NV_0 \frac{d^2E_0(V)}{dV^2}|_{V_0} \tag{35}$$

In this relation, the energy of atom individually is, in fact, positive and equal to $+E_0$.
We can have for free energy the following relationship;

$$E = E|_{T=0}+E_{Oscillation} \tag{36}$$

In which;

$$E = U - TS \tag{37}$$

At T=0;

$$E|_{T=0} = U \tag{38}$$

Therefore (36) becomes;

$$E = -NE_0\ (V)+E_{Oscillation} \tag{39}$$

For a linear oscillator we can write;

$$E= -KT\ LogZc \tag{40}$$

Free energy of solid of volume V, can be deduced as following;

$$E = N\,[-E_0(V)+3KT\,Log\ \frac{X_0(V)}{\pi KT}\ \frac{\sqrt{E_0(V)}}{2m_0}] \tag{41}$$

Now the literal expression of the solid can easily be obtained;

$$P = \frac{\partial E}{\partial T}|T \tag{42}$$

$$P \approx N\frac{dE_0(V)}{dV} - \frac{3NKT}{X_0}\ \frac{dX_0(V)}{dV} \tag{43}$$

If the pressure becomes zero P=0, then;

$$N\frac{dE_0(V)}{dV} - \frac{3NKT}{X_0}\ \frac{dX_0(V)}{dV} \tag{44}$$

Knowing that;

$$\frac{dE_0(V)}{dV}(V-V_0)\frac{d^2E_0(V)}{dV^2}|_{V_0}+\dots \tag{45}$$

Combining (44) and (45), yields;

$$\frac{V-V_0}{\chi_0 V_0} = -3NKT\frac{d}{dV}LogX_0|v_0 \tag{46}$$

(46) can be written as following;

$$-\frac{d}{dV}LogX_0|_{V_0} = \frac{\beta_0 V_0}{\chi_0 C_v} = \gamma \tag{47}$$

β_0 is the dilatation coefficient at zero pressure and C_v the specific heat of solid.

In order to get the variation of compressibility as a function of temperature near the equilibrium position, defined by volume V_0, we can have;

$$\chi = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T \quad (48)$$

As the solid has very small compressibility, then we can have;

$$1/\chi = -V_0\frac{\partial P}{\partial V}\Big|_T = -N V_0 \frac{d^2E_0}{dV^2}\Big|_{V_0} + 3NKT V_0 \frac{d^2 \mathrm{Log} X_0}{dV^2}\Big|_{V_0} \quad (49)$$

First derivation of (49) yields;

$$\frac{d\chi}{dT} = \frac{-\chi\beta_0 V_0^2}{\gamma} \frac{d^2 \mathrm{Log} X_0}{dV^2}\Big|_{V_0} \quad (50)$$

As, $d\chi/dT$, is negligible, then we can have;

$$\frac{d\mathrm{Log}\chi}{dT} = -\frac{\beta_0 V_0^2}{\gamma} \frac{d^2 \mathrm{Log} X_0(V)}{dV^2}\Big|_{V_0} \quad (51)$$

Numerical application: case of aluminium: For aluminum, we have the experimental values such as:

$$\frac{d\mathrm{Log}\chi}{dT} = 5.5\times10^{-4}(^0K)^{-1} = \mathrm{Cte},\ \beta_0 = 6.78\mathrm{x}10^{-5}\ (^0K)^{-1},$$

$$\chi\,(300°K) = 1.37\mathrm{x}10^{-11}\ m^2/N$$

$V=1.003\mathrm{x}10^3\ m^3$

These data yield for γ, δ, the numerical values as;

$$-\frac{d}{dV}\ \mathrm{Log}X_0\Big|_{V_0} = \frac{\beta_0 V_0}{X_0 C_v} = \gamma = 2.17$$

$$\delta = -V_0^2 \frac{d^2 \mathrm{Log} X_0}{dV^2}\Big|_{V_0} = 1.76$$

Where;

$$-\frac{V_0^2}{X_0}\frac{d^2 X_0}{dV^2}\Big|_{V_0} = 12.9$$

δ is, in fact, the Gruneisen constant.

If $X_0 = K\mu^{-1/6}\chi^{-1/2}$ where K is a constant, μ is specific mass and χ is the compressibility, it can be easily seen that the following state equation, is a solution near the equilibrium, which is defined by the volume V_0;

$$(V_0-V)/V_0 = AP-BP^2 \quad (52)$$

The first derivative of (52), yields;

$$dV = V_0(2PB-A)dP \quad (53)$$

Considering the equations (38), (45) and (48), we can deduce;

$$(V_0-V)/V_0 = \chi_0\,P - 2.34\,\chi^2\,P \quad (54)$$

As the solid is of small compressibility therefore, for all the range of temperature, the state equation can be given by following equation;

$$(V_0-V)/\chi(T)V_0 = P-2.34\chi(T)\,P^2 \quad (55)$$

RESULTS AND DISCUSSION

The concept of considering atom as a linear oscillator, offered a simple classical model for study of solids. One-dimensional oscillation of atom has been considered. Atom itself was considered as a point of mass and was subjected to move along X-axis. This simplification made the partition function be easily solved and with a reasonable assumption its simplified expression has been established and linear oscillator Hamiltonian was also expressed and hence the mean energy of such linear oscillator was deduced.

An expression for compressibility has been established and finally the necessary work for compressing a solid, from its volume at zero Kelvin to any volume at any temperature, as a function of compressibility factor and temperature was established. A literal expression for the pressure applied to solid and also an expression showing the compressibility variation have been deduced.

As a numerical application, aluminum has been chosen for which,γ, the Gruneisen constant and δ, have been calculated. U=Kt is not valid in our model unless at high temperature, which limits our model. On the other hand, χ_0, is actually depending on the frequency V_0, of the studied linear oscillator, therefore Einstein model can be used for solid study with better precision. In addition, quantum mechanics generalize the classical study results for all temperatures while classical study offers less complexity in obtaining results and much simplicity in calculations.

This study showed that a classical model with an aspect of linear oscillation of the atom can be applied for study of solids. Simple assumptions were considered in order to establish relations for compressibility coefficient, pressure applied to solid and Gruneisen constant. The model was well applied to aluminum as solid in order to find out the physical parameters. The model has a simplicity for calculation and can be used for all metals as solids.

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