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Thermoelastic properties of materials under high temperature using equation of state

Jeewan Chandra[1]*, Kuldeep Kholiya[2], Pooja K.Bhatt[3]

[1]Department of Physics, National Institute of Technology Uttarakhand, (INDIA)

[2]Department of Applied Science, B.T. Kumaon Institute of Technology, Dwarahat, (INDIA)

[3]Kumaun University Nainital, (INDIA)

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E-mail : jeewan25may@rediffmail.com

ABSTRACT

The purpose of present study is to show first time the applicability of Singh and Gupta's integral form of equation of state not only for the Bulk materials but nanomaterials as well. This Equation is based on some mathematical technique and used to analyze the temperature dependence of thermal expansion coefficient, relative volume change and isothermal bulk modulus. We are taking metals Ag and Au as bulk materials and fullerene (C_{60}) as a nanomaterial. There is found an excellent agreement of our calculated values with the experimental data, which proves the validity of Singh and Gupta's equation of state for both bulk materials and nanomaterials on equal potential.

KEYWORDS

Nanomaterial;
Thermal expansion;
Equation of state.

INTRODUCTION

The Study based on the EOS at high-pressure and high temperature is of fundamental interest because they permit interpolation and extrapolation in to the regions in which the experimental data are not available adequately. They help in planning future high-pressure experiments, and are also important in comparing static high-pressure experiments with shock wave experiments, in which the treatment of thermal effect is particularly important. Some high-pressure experimental techniques are also available for high-pressure high temperature study at laboratory, which are Synchrotron X-Ray diffraction and spectroscopy, Raman scattering, Laser heating, Brillouin scattering and Multi-anvil synthesis. Understanding of metallic properties at high-pressure and high temperature is a central problem of high-pressure physics. Basically metals are structurally distinguished from non-metals by their atomic bonding and electron availability. The free electron is lost from the outer shell of metallic atoms are available to carry the electricity and heat capacity.

Over the past decade, nanomaterials have been the subject of enormous interest. These materials, notable for their extremely small size, have the potential for wide-ranging industrial, biomedical, and electronic applications. Nanomaterials can be metals, ceramics, polymeric materials, or composite materials. Nanocrystalline materials with particle size of 1-100 nm are of current interest because they show noble physical and chemical

properties that may differ from those of the corresponding bulk materials

In the 1985, hollow carbon nanospheres were discovered. These spheres were called buckyballs or fullerenes, in honor of architect and futurist Buckminster Fuller, who designed a geodesic dome with geometry similar to that found on the molecular level in fullerenes[1].The basic C_{60} structure consists of 60 carbon atoms that link together to form a hollow cage-like structure. The structure consists of 32 faces of which 20 are hexagons and 12 are pentagons. Of these, no two pentagons share a vertex. Several physical properties such as compressibility[2], bulk modulus[3] and Debye temperature[4] have been studied for bulk fullerenes C_{60} but less literature is available for a single fullerene $C_{60.}$

METHOD OF ANALYSIS

It has been noted that under the effect of temperature the product of thermal expansion coefficient and bulk modulus remains constant[5], i.e.

$$\alpha K_T = \textbf{Constant.} \quad (1)$$

Where α is volume thermal expansion coefficient and K_T is bulk modulus.

On differentiating equation (1) with respect to T, at constant pressure, we have

$$\alpha\left(\frac{dK_T}{dP}\right)_P + K_T\left(\frac{d\alpha}{dT}\right)_P = 0 \quad (2)$$

$$\textbf{or}\ \left(\frac{dK_T}{dT}\right)_P = -\frac{K_T}{\alpha}\left(\frac{d\alpha}{dT}\right)_P \quad (3)$$

The Anderson Gruneisen parameter δ_T is defined as

$$\delta_T = -\frac{1}{\alpha K_T}\left(\frac{dK_T}{dT}\right)_P \quad (4)$$

Substituting the value of equation (3) in equation (4) we get

$$\delta_T = \frac{1}{\alpha^2}\left(\frac{d\alpha}{dT}\right)_P \quad (5)$$

Here α is defined as

$$\alpha = \frac{1}{V}\left(\frac{dV}{dT}\right)_P \quad (6)$$

From equation (6) and (5) we get

$$\delta_T = \frac{V}{\alpha}\left(\frac{d\alpha}{dV}\right)_P \quad (7)$$

Gruneisen parameter is basically a measurement of anharmonicity in a crystal.Recent studies revealed that δ_T changes with temperature and it must be considered as a temperature – dependent parameter. The temperature dependence of δ_T[6] is given by the following empirical relationship

$$\delta_T = \delta_T^0 x^k \quad (8)$$

where $X= (T/T_0)$, T_0 is reference temperature (room temperature) and δ_T^0 is the value of Anderson Gruneisen parameter (δ_T) at $T= T_0$ and k is new dimensionless thermo elastic parameter, whose value is calculated by the slope of the graph plotted between $\log(\delta_T)$ and $\log(T/T_0)$.

So the value of k is defined as

$$k = \left(\frac{\partial \ln \delta_T}{\partial \ln X}\right) \quad (9)$$

Substituting equation (8) in equation (5) we get

$$\delta_T^0 X^k = \frac{1}{\alpha^2}\left(\frac{d\alpha}{dT}\right)_P.$$

or

$$\delta_T^0\left(\frac{T}{T_0}\right)^k = \frac{1}{\alpha^2}\left(\frac{d\alpha}{dT}\right)_P \quad (10)$$

Integrating equation (10)

$$\frac{\delta_T^0}{T_0^k}\left(\frac{T^{k+1}}{k+1}\right) = -\frac{1}{\alpha_T} + C, \quad (11)$$

where C is integrating constant, which can be calculated from initial condition at $T=T_0$ and $\alpha = \alpha_0$.

$$C = \frac{\delta_T^0 T_0^{k+1}}{T_0^k(k+1)} + \frac{1}{\alpha_0} \quad (12)$$

Using equation (12) with (11) we have

$$\frac{\delta_T^0}{T_0^k}\left(\frac{T^{k+1}}{k+1}\right) - \frac{\delta_T^0}{T_0^k}\left(\frac{T_0^{k+1}}{k+1}\right) = \frac{1}{\alpha_0} - \frac{1}{\alpha_T}.$$

Rearranging we get final expression for volume thermal expansion coefficient (α_T).

$$\alpha_T = \alpha_0\left[1 - \frac{\delta_T^0\alpha_0}{T_0^k(k+1)}\left\{T^{k+1} - T_0^{k+1}\right\}\right]^{-1} \quad (13)$$

Where α_0 is the thermal expansion coefficient at reference temperature T_0. this equation requires only three input parameter α_0, δ_T^0 and k at room temperature and the value of α_T is evaluated directly as a function of

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temperature. The empirical temperature dependence of δ_T is assumed then according to equation (4) at P=0, may also rewritten as

$$-\left(\frac{dK_T}{dT}\right) = \alpha_0 K_0 \delta_T \quad (14)$$

Using equation (8)

$$-\left(\frac{dK_T}{K_0}\right) = \alpha_0 \delta_T^0 \left(\frac{T}{T_0}\right)^k dT \quad (15)$$

Integrating above equation (15), we get

$$K_T = -\frac{\alpha_0 K_0 \delta_T^0}{T_0^k}\left(\frac{T^{k+1}}{k+1}\right) + C, \quad (16)$$

Where C is integrating constant, which can be calculated by initial conditions $T=T_0$, and $K=K_0$.

We get the final expression for bulk modulus K_T is

$$K_T = K_0\left[1 - \frac{\alpha_0 \delta_T^0}{T_0^k (k+1)}\left\{T^{k+1} - T_0^{k+1}\right\}\right] \quad (17)$$

The expression for the volume thermal expansion (V/V_0) can be obtained by making use of the following equation

$$dK_T = -\delta_T K_T \frac{dV}{V} \quad (18)$$

Differentiating equation (17) with respect to temperature, we get

$$dK_T = -\frac{\alpha_0 K_0 \delta_T^0}{T_0^k} T^k dT \quad (19)$$

Using equation (19) with equation (18) we get

$$\frac{dV}{V} = \frac{\alpha_0}{\left[1 - \frac{\alpha_0 \delta_T^0}{T_0^k (k+1)}\left\{T^{k+1} - T_0^{k+1}\right\}\right]} dT \quad (20)$$

Integrating equation (20) we get the final expression for volume thermal expansion (V/V_0) as follows

$$\frac{V}{V_0} = \exp\left[\int_{T_0}^{T} \frac{\alpha_0}{\left[1 - A\left\{T^{k+1} - T_0^{k+1}\right\}\right]} dT\right], \quad (21)$$

where $A = \frac{\alpha_0 \delta_T^0}{T_0^k (k+1)}$.

The equation (21) is known as Singh and Gupta equation of state for the volume thermal expansion.

The value of dimensionless thermoelastic parameter k can be estimated from the slope of the graph plotted between $\log\delta_T$ and $\log T/T_0$. The values of δ_T and δ_T^0 have been calculated from equation (5).

TABLE 1 : Input parameters at room temperature. Volume thermal expansivity α_0 (in unit of $10^{-5}K^{-1}$), bulk modulus K_0 (in GPa) and first derivative of bulk modulus K_0' are taken from as indicated in square bracket.

Metals	α_0 (10^{-5} K^{-1})	K_0 (GPa)	δ_T^0	k	K_0'
Ag	5.76[7]	99.6[8]	6.30	-0.068	6.20[9]
Au	4.23[7]	166.6[8]	7.80	-0.005	5.10[9]
C_{60}	1.727[11]	491[10]	122	-1.34	-

RESULTS AND DISCUSSION

The values of Thermal expansivity (α_T), isothermal bulk modulus (K_T) and volume thermal expansion (V/V_0), at different temperatures and atmospheric pressure have been calculated from equations (13, 17, 21) respectively, for Au, Ag and fullerene. The variation of

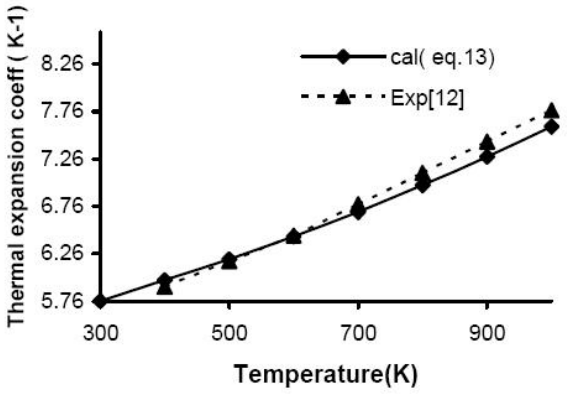

Fig1: Thermal expansion coefficient Vs Temperature for Ag

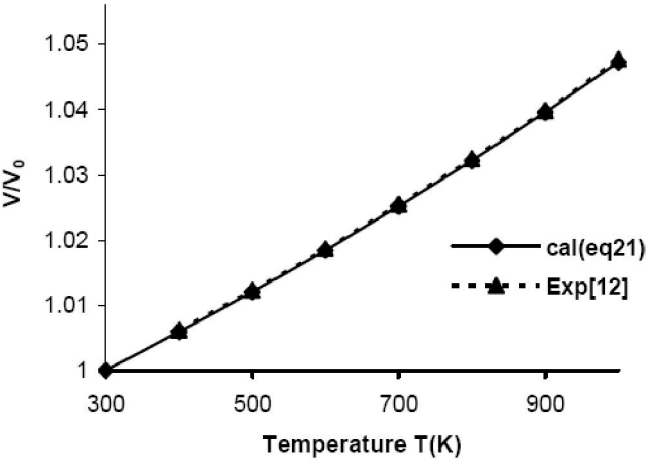

Fig2: V/V_0 Vs Temperature for Ag

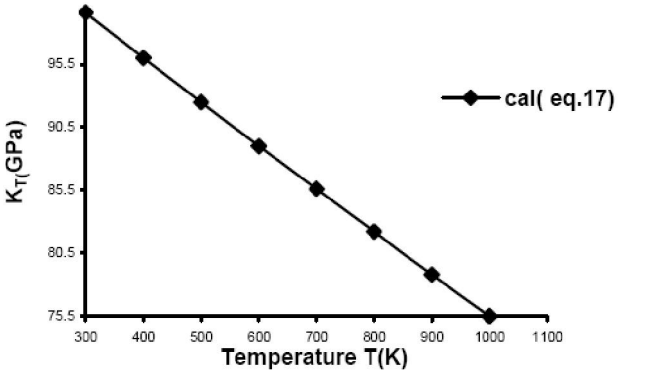

Fig3: Isothermal Bulk modulus Vs Temperature for Ag

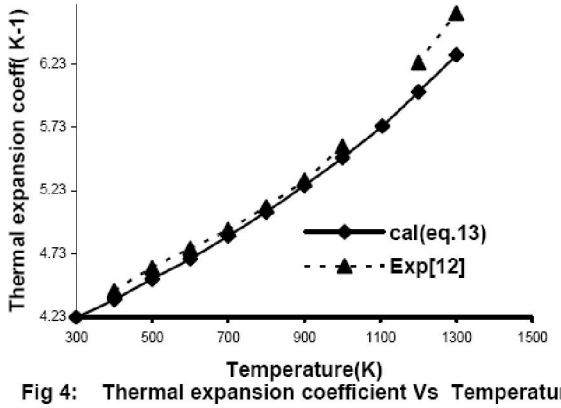

Fig 4: Thermal expansion coefficient Vs Temperature for Au

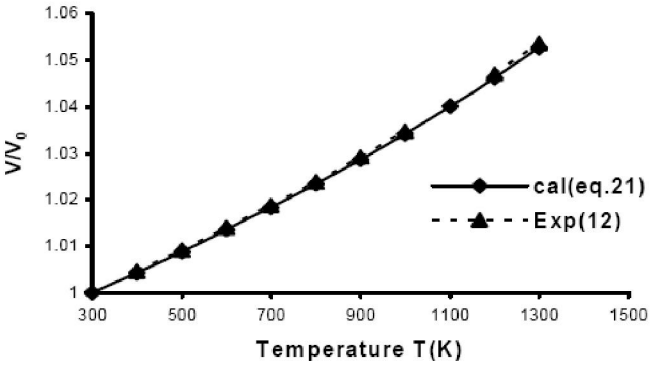

Fig 5: V/V_0 Vs Temperature for Au

thermal expansivity (α_T), bulk modulus (K_T) and volume thermal expansion (V/V_0) of these materials are shown in Figure (1-9), together with available experimental values[11, 12] for the sake of comparison of our results. It is observed from the graphs that the values of It is found in each case that our calculated values are in close agreement with the experimental data. Thus it is predicted here that the Singh and Gupta's integral form of equation of state which is used to determine the elastic properities of solids under the effect of temperature, is not only applicable for bulk materials but nanomaterials also with equal footing.

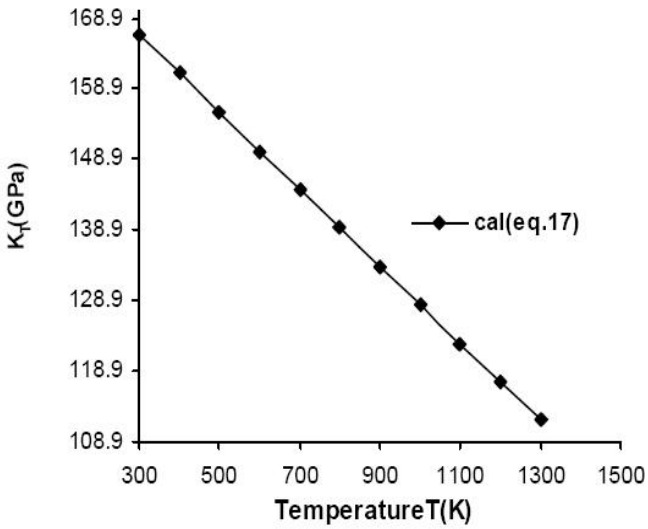

Fig 6: K_T Vs Temperature for Au

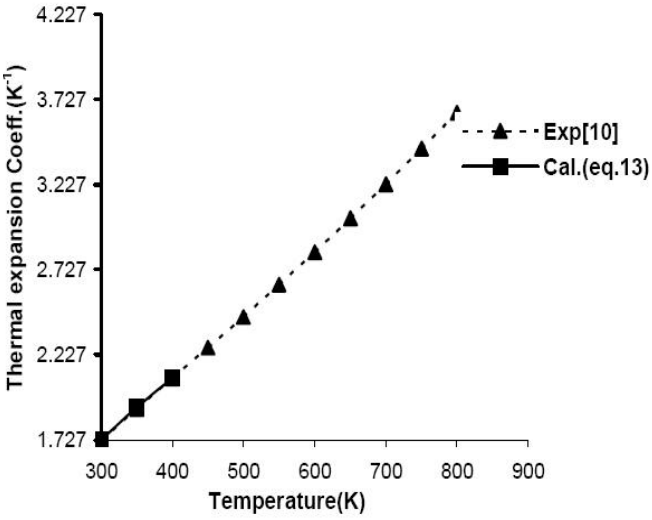

Fig 7: Thermal expansion coeff. Vs temperature for fullerene

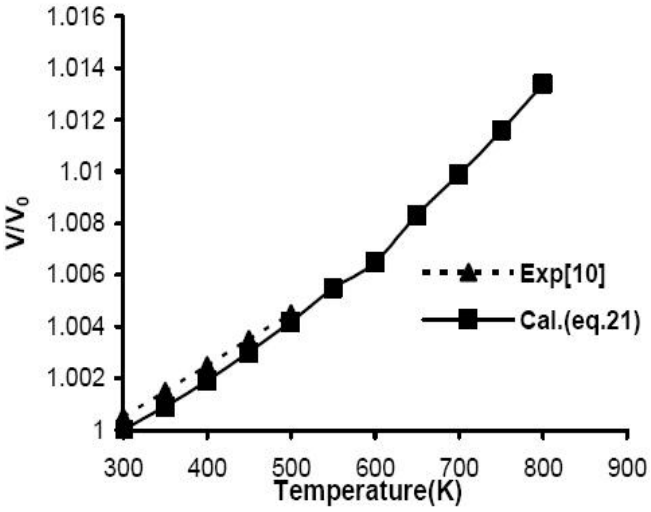

Fig8: V/Vo Vs temperature for fullerene

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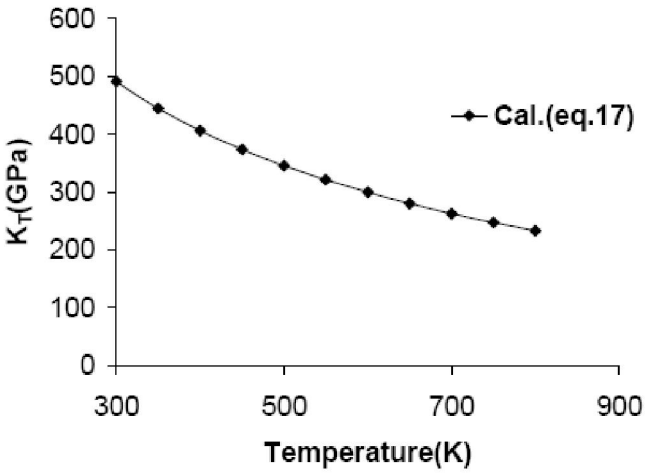

Fig 9: K_T Vs Temperature(K) for Fullerene

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