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Comparative study of compression in fullerites and carbon nanotubes under high pressure

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ABSTRACT

In the present study, an analysis of high pressure compression in fullerites such as C_{60}, C_{70},C_{84} and Carbon nanotubes has been performed using the two parameter based isothermal equations of state,i.e. Murnaghan equation, Kumar equation, Vinet equation, Suzuki equation, Sharma equation and usual Tait's equation. The results achieved from these equations are compared with the available experimental data. It is found that the results obtained from usual Tait's equation of state are in close agreement with the experimental data as compared to those calculated from other equations of state. A good agreement between theory and experiment demonstrates the validity of the Tait's equation of state in nanostructured fullerites and nanomaterials as in case of bulk materials.

KEYWORDS

Nanomaterials;
Equations of state;
Compression;
Isothermal bulk modulus.

INTRODUCTION

The nanomaterials are very sensitive to external parameters like pressure and temperature. The study of nanomaterials under high pressure is considered as a possible path to expand the range of available solid state materials. High pressure applications have the potential for the exploration of infinity of paths for nanoassembling or phase transformation in a controlled way and constitute a unique route for the elaboration of new materials[1, 2].

Fullerenes are the nanomaterials made of carbon atoms. They have been the focus of attention to many scientific groups after their preparation in solid state by Kratschmer et al. in1990[3]. Blank et al. in 1997[4] studied the physical properties of super hard and ultra hard fullerites synthesized from solid C_{60} by high pressure and high temperature treatment and showed that properties of fullerites are different from diamond and other carbon form. Duclos et al. 1991[5] performed the experimental measurements of solid C_{60} up to 200 kbar pressure at room temperature. Duclos[5] used Birch Murnaghan equation of state (BMEOS) and Vinet equation to fit the experimental data. It has been observed that no notable change in the bonding character of solid C_{60} takes place up to 200 kbar. Another fullerite solid C_{70} consisting of 70 atoms of Carbon is also found in abundance. Christides et al.[6] observed the structure of solid C_{70} under pressure at ambient temperature to 25 GPa using energy dispersive X-ray diffraction (EXRD). The elastic and microstructural properties of C_{60} and C_{70} based on polymerized

fullerites have been studied by Prokhorov et al. in 2002[7] under pressure up to 15 GPa and elevated temperature. Margiolaki in 2002[8] investigated the pressure dependence of C_{84} solid. At room temperature and up to 9.24 GPa pressure, no evidence of phase transition is found and the structure of C_{84} remains FCC. Further, the carbon nanotubes (CNT) have been the subject of interest for researchers because of their unique electronic and mechanical properties. In 1996, Iijima et al.[9] noted that their circular sections can be deformed and even collapsed as induced by the external forces, local bents or defects, or by vander waal forces. Tang et al.[10] reported that Single walled carbon nanotube (SWCNT) show linear elastic behavior up to 1.5 GPa pressure at room temperature. The volume compressibility of SWCNT measured using X-ray diffraction was 0.024 GPa. Theoretical analysis suggests that the intertubular gap is reduced in single-walled carbon nanotubes on applying pressure. Reich and Thomson[11] have used the first principle method, i.e., ab-initio method and calculated the bulk modulus of CNT as 37 GPa to be nearly the same as that of graphite. Kwon et al. (2004)[12] examined fullerenes and carbon nanotubes under varying temperature and studied the shape changes in them using molecular dynamics simulations.

It is found that the compressional behavior of fullerites and carbon nanotubes under pressure have been widely investigated experimentally in the high pressure research field. However, the theoretical work in this field especially in nanostructured fullerites has not been explored adequately. Therefore, it may be useful to present a simple theoretical approach to study the high pressure behavior of nanomaterials and fullerites. The method of analysis is given in section 2. The results and discussions are given in section 3 and section 4 deals with the conclusion of the research work.

METHOD OF ANALYSIS

Under the research of high pressure physics, the Tait's equation is based on the assumption that the product of coefficient of thermal expansion (α_T) and bulk modulus (B_T) is constant under the effect of pressure[13], i.e.

$$\alpha_o B_o = \alpha_T B_T = constant \quad (1)$$

On differentiating equation (1) relative to volume V at temperature T, we get:

$$\alpha\left(\frac{dB}{dV}\right)_T + B\left(\frac{d\alpha}{dV}\right)_T = 0 \quad (2)$$

Anderson – Gruneisen parameter is given by:

$$\delta_T = \frac{V}{\alpha\left(\left[\frac{d\alpha}{dV}\right]\right]_T} \quad (3)$$

where δ_T is Anderson – Gruneisen parameter at constant temperature T.

Using equations (2) and (3), we get:

$$\delta_T = \frac{V}{\alpha(\,[\![\,d\alpha/dV)\,]\!]_{\downarrow}T} = -V/B\,(dB/dV)_{\downarrow}T \quad (4)$$

Assuming δ_T to be independent of V, Anderson – Gruneisen parameter is found equal to B_o';

$$\delta_T = \left(\left[\frac{dB}{dP}\right]\right]_T = B_o' \quad (5)$$

Anderson- Gruneisen parameter and $\eta = V/V_o$ (where V_o is the initial volume) are related by the following relation[13],

$$\left(\frac{\delta_T + 1}{\eta}\right) = A \quad (6)$$

where A is a constant.

The bulk modulus B is equal to:

$$B = -V\left(\frac{dP}{dV}\right)_T \quad (7)$$

From above equation (7),

$$\frac{B}{B_o}\exp A\left[1 - \frac{V}{V_o}\right]dV = -dP \quad (8)$$

The integration of equation (8) gives

$$P = \frac{B_o}{A}\left[\exp A\left\{1 - \frac{V}{V_o}\right\} - 1\right] \quad (9)$$

Here is the initial bulk modulus at pressure P=0 and V= V_o.

A is evaluated at V= V_o as follows:

$$A = B_o' + 1 \quad (10)$$

On substitution of constant A in equation (9), Usual Tait's equation of state obtained in terms of pressure P is as follows:

$$P = \frac{B_o}{(B_o' + 1)}\left[\exp(B_o' + 1)\left\{1 - \frac{V}{V_o}\right\} - 1\right] \quad (11)$$

The bulk modulus corresponding to usual Tait equation (11) at constant temperature is given by:

$$\frac{B_T}{B_o} = \frac{V}{V_o}\left[\exp(B_o' + 1)\left\{1 - \frac{V}{V_o}\right\}\right] \quad (12)$$

where V is the volume of the material at pressure required to compress it, keeping the temperature constant. V_o is the initial volume at room temperature T_o.

Murnaghan defined in his general theory of finite strain[13] that bulk modulus varies linearly with pressure. Murnaghan equation is given as follows:

$$P = \frac{B_o}{B_o'}\left[exp\left\{-B_o' ln\left(\frac{V}{V_o}\right)\right\} - 1\right] \quad (13)$$

Later, Kumar[14] expanded the Murnaghan equation MEOS up to the nearest neighbor and wrote the equation in the following form:

$$P = \frac{B_o}{B_o'}\left[\left\{\exp B_o'\left(1 - \frac{V}{V_o}\right) - 1\right\}\right] \quad (14)$$

Vinet EOS used to study some properties of solids and nanomaterials reads as follows[15]:

$$P = \frac{3(1-\chi)B_o[\exp \eta(1-\chi)]}{\chi^2} \quad (15)$$

where $\eta = \frac{3(B_o' - 1)}{2}$ and $\chi = \left(\frac{V_o}{V}\right)^{\frac{1}{3}}$ (16)

Suzuki formulation is based on Gruneisen theory by San-Miguel and Suzuki[16]:

$$P = B_o\left(1 - \frac{V}{V_o}\right) + B_o\left(\frac{B_o' - 1}{2}\right)\left(1 - \frac{V}{V_o}\right)^2 \quad (17)$$

In terms of Bulk modulus as a function of volume compression Suzuki equation reads as follows:

$$\frac{B_P}{B_0} = \left[\frac{V}{V_0}\left\{1 + (B_0' - 1)\left(1 - \frac{V}{V_0}\right)\right\}\right] \quad (18)$$

The size dependent equation of state (EOS) for nanomaterials in terms of pressure P formulated by Sharma and Kumar[17] is as follows:

$$P = B_o\left(1 - \frac{V}{V_o}\right) + B_o\left(\frac{B_o' + 1}{2}\right)\left(1 - \frac{V}{V_o}\right)^2 \quad (19)$$

Equation (19) thus relates pressure and volume compression (V/V_o). The Mie-Gruneisen theory of EOS supports equation (19) and reproduces the Shanker EOS[18].

In terms of Bulk modulus as a function of volume compression Sharma and Kumar equation reads as follows:

$$B = B_0\left(\frac{V}{V_0}\right)\left[1 + (B_o' + 1)\left\{1 - \frac{V}{V_o}\right\}\right] \quad (20)$$

RESULTS AND DISCUSSION

In the present investigation, volume compression in fullerites and carbon nanotubes are determined under the effect of high pressure by making use of different isothermal equations of state, i.e. usual Tait's equation (11), Murnaghan equation (13), Kumar equation (14), Vinet equation (15), Suzuki equation (17) and Sharma equation (19).The equation of state employed in the present study consists of , viz. B_o and B_o'. The compiled data are given in TABLE 1 along with their proper references.

Using eq. (11), eq. (13), eq. (14), eq. (15), eq. (17) and eq. (19); compressional behavior in fullerites and carbon nanotubes is determined and the results are shown in Figures 1-5 along with the experimental data for the sake of comparison. It is found that the usual Tait equation (11) yields close better agreement with the experimental values for both fullerites and nanotubes especially at lower pressure range. The percentage deviation in volume compression at highest pressure for fullerites and Carbon nanotubes are reported in TABLE 2 which demonstrates the validity of Tait eq. (11) in the present work.

It is found that the results obtained by Usual Tait's equation (eq.11) are certainly in good agreement with the available experimental data. Since the results obtained by Usual Tait's equation (eq.11) are in good agreement with the available experimental data, the variation of bulk modulus B with pressure is also

TABLE 1 : Input data used in the present work

S.No.	Materials	B_o (GPa)	B_o'	Ref.
1.	C_{60}	18.1	5.7	[5]
2.	C_{70}	25	10.6	[6]
3.	C_{84}	20	16.1	[8]
4.	Carbon Nanotube individual	230	4.5	[10]
5.	Carbon Nanotube Bundle	37	11	[11]

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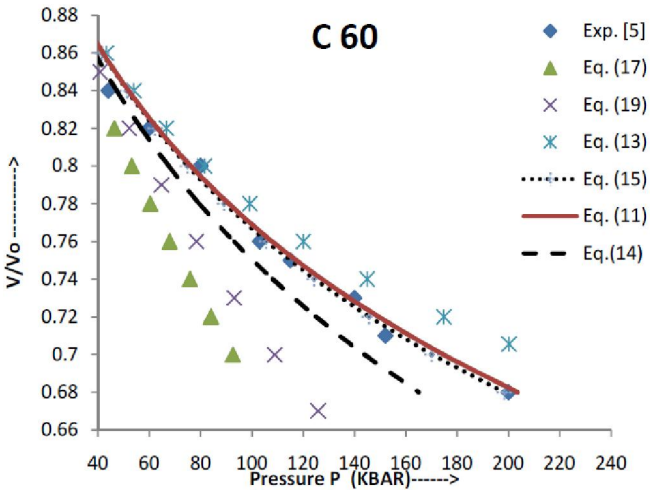

Figure 1 : Variation in volume compression vs. pressure in C_{60}

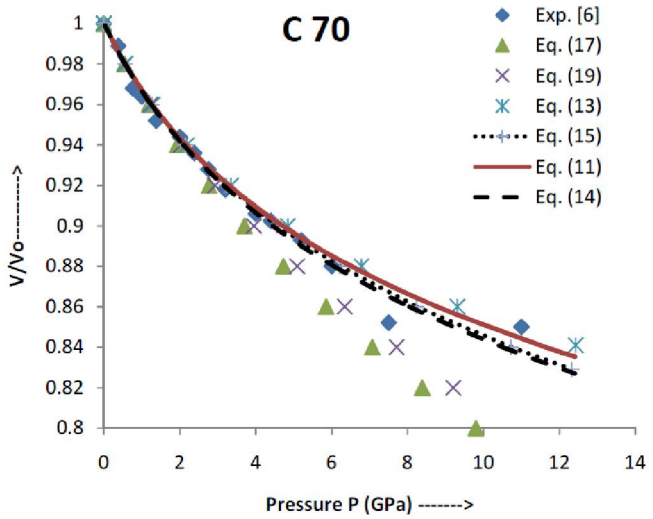

Figure 2 : Variation in volume compression vs. pressure in C_{70}

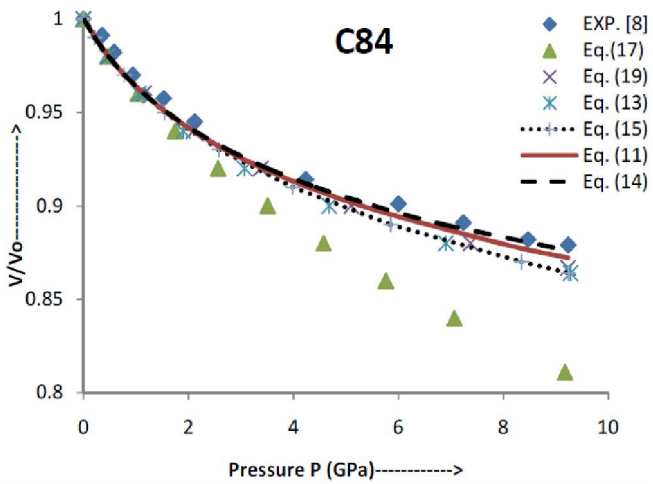

Figure 3 : Variation in volume compression vs. pressure in C_{84}

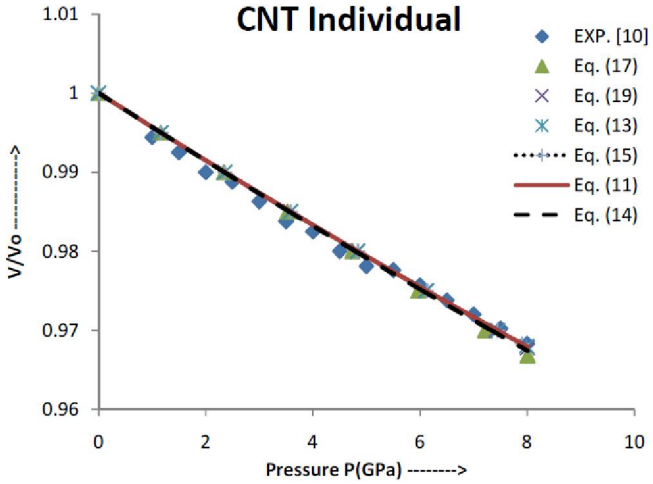

Figure 4 : Variation in volume compression vs. pressure in CNT Individual

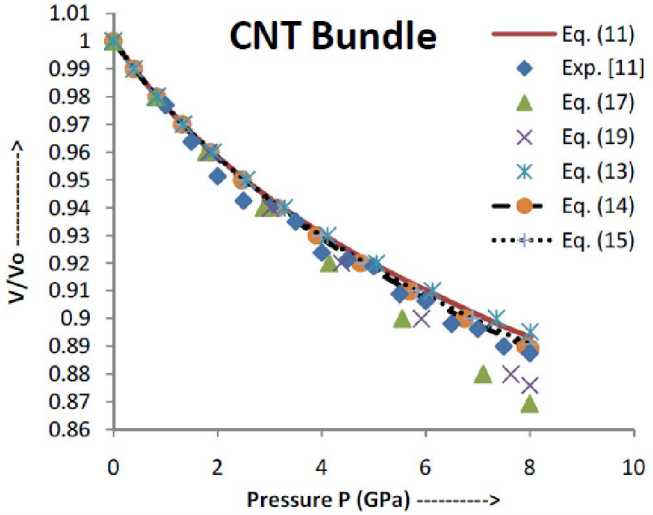

Figure 5 : Variation in volume compression vs. pressure in CNT Bundle

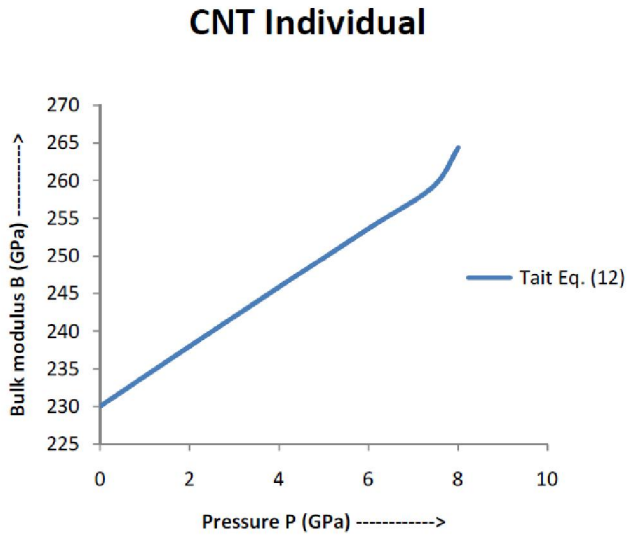

Figure 6 : Variation in bulk modulus vs. Pressure P in CNT individual

TABLE 2 : Percentage deviation in volume compression using different equations of state

Materials	Eq.(13)	Eq.(14)	Eq. (15)	Eq.(17)	Eq.(19)	Eq.(11)
C_{60}	3.75	4.26	0.15	27.2	18.3	0.29
C_{70}	1.86	3.50	3.27	10.61	7.58	2.50
C_{84}	0.345	1.70	1.70	7.84	6.82	0.77
CNT individual	0.041	0.092	0.041	0.154	0.051	0.04
CNT bundle	0.84	0.169	0.361	2.07	1.29	0.642

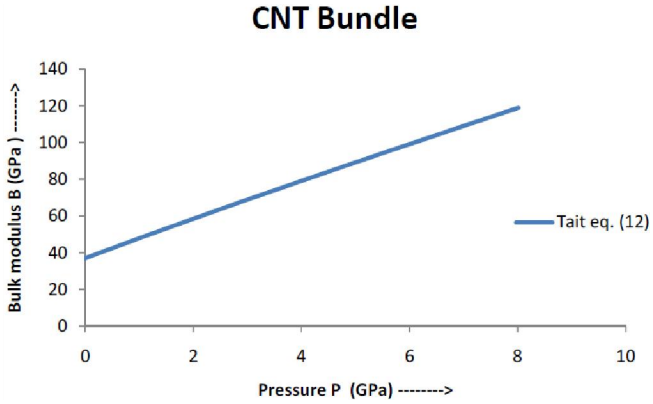

Figure 7 : Variation in bulk modulus vs. pressure P in CNT bundle

evaluated using eq. (12) in carbon nanotube individual and carbon nanotube bundles. The results obtained by Usual Tait's equation of state (12) are shown in Figures 6 and 7. It is clear from Figures 6 and 7 that the bulk modulus increases on applying pressure in Carbon nanotubes and thus they become more rigid with pressure. On the basis of overall description, it may be emphasized here that the present approach is capable of explaining the compressional behavior of fullerites and nanotubes under high pressure satisfactorily and more accurately.

CONCLUSIONS

In the present research work, the Usual Tait's EOS (eq. 11) is found to be the most suitable equation for the study of mechanical properties of fullerites and carbon nanotubes. Because of the simplicity and applicability of the Tait's equation of state, this may be of the current interest to the researchers engaged in the study of elastic properties of fullerites and carbon nanotubes under high pressure. The main advantage of the equation of state is that it satisfies the basic laws of thermodynamics with regard to relations at high pressure and also provides extrapolated values in regions where experimental values are not available.

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