RESEARCH PAPER

Study of Compression in C_{60}, C_{70}, C_{84} and CNT under High Pressure by Using Bulk and Nano EOSs

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ABSTRACT

The variation of V/V_o for nano C_{60}, C_{70}, C_{84}, and CNT against high pressure has been evaluated using Vinet and Birch-Marnghan EOSs as well as Nano EOSs. Different equations' outputs were compared to experimental data as well as to each other. The compatibility of the various EOS results suggests that the EOSs of bulk materials may be applied to the computations of nanoparticles. Calculations of bulk modulus fluctuations under high pressure for C_{60}, C_{70}, C_{84}, and CNT Materials showed a viable use for bulk EOSs. and nano materials except Birch-Marnghan EOS.

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INTRODUCTION

The researches of high pressure have been participated in the development of science and technology. The equation of state (EOS) which temperature and volume-pressure relationships is of great importance in such studies as it used to determine many properties of bulk and nano-materials under varying pressure and temperature conditions [1].The wide range applications of carbon nanomaterials in many aspects of life gave a push to researchers around the world to work hard and continuously to develop these nanomaterials and their fabrication techniques [2]. The properties of nanomaterials which are in the range from 1-100 nm of size, are quietly different from that of bulk- materials .The investigations of nano-materials under high pressure can add useful information and best understanding of these materials since they are infinitesimally small in size so high pressure's affect will be significant on their properties.One of the methods used to introduce modifications to the configuration and structure of nano-particles is by applying high pressure on these particles. The application of mathematical extrapolation and interpolation to the unreachable regions by actual observations is made possible by theoretical studies utilizing EOSs under high pressure.

For this study, we used customized EOSs for nanomaterials and other EOSs for bulk materials to assess how high pressure will affect Nano C_{60},C_{70},C_{84} and CNT [3-4]. All of the EOS's obtained results were compared to experimental data. Additionally, research into bulk modulus change

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under high pressure is a potential method for developing a universal EOS for solids.

THEORETICAL EOS

The three classes that comprise the EOSs of materials are as follows:

1- Birch-Murnaghan EOS (P_{BM}) (Eq. 1) [6]. Where, P- pressure, B_0- isothermal bulk modulus in the ambient state B_0' - pressure's first derivative of B_0, V- high-pressure volume, V_0- (atmospheric) pressure volume.

2- Vinet EOS (P_v) (Eq. 2) [7].

3- EOS based on assumption about the relationships between its variables, as Murnaghan EOS (Eq. 3) [8]. Where, P_M –Murnaghan EOS, B_{os} - adiabatic bulk modulus at ambient conditions, B'_{os} - pressure's first derivative of B_{os}.

The volume expansion of nanomaterials at high pressure was studied by (Singh et al.2012) [3] using an easy EOS derived from the concept of bulk modulus. The bulk- modulus and its first pressure derivative are the only two input variables required for calculations (Eq. 4). Where, P_s- represent Singh EOS.

Singh and Kao [4] revised equation (4) based on the Mie-Grüneisen EOSs theory, which stipulates the following definition of pressure including thermal pressure (P_{th}) and lattice potential energy (U) (Eq. 5 and Eq. 6). Where, P_{s-k} - EOS by Singh - Kao. This derivation adduced Eq. 4 validity.

On the basis of the constant value for the product of the thermal expansion coefficient (α) and the isothermal bulk- modulus (B_T) under pressure, Kholiya and Chandra developed equation (4). Kholiya and Chandra [5]. They proposed in their paper that the first pressure derivative of the bulk- modulus be set to value 4. Bearing in mind that the fewer input parameters, the better the EOSs. So, Eq. 7 turned to be one parameter EOSs as B_0. Where, P_{C-K} – EOS by Chandra and Kholiya.

Isothermal bulk- modulus (B_T)

From the definition of bulk- modulus, according to certain increase in pressure there will be a volume compression calculated in fundamental units of pressure such as Pascal. Thermodynamically, the bulk- modulus can be expressed by the Eq. 8.

The change in bulk-modulus caused by high pressure is regarded to be a step toward developing a general equation of state for solids

$$P_{BM} = \frac{3B_0}{2}\left[\left(\frac{V}{V_0}\right)^{-\frac{7}{3}} - \left(\frac{V}{V_0}\right)^{-\frac{5}{3}}\right]\left[1 + \frac{3}{4}(B_0' - 4)\left(\left(\frac{V}{V_0}\right)^{-\frac{2}{3}} - 1\right)\right] \quad (1)$$

$$P_V = 3B_0\left(\frac{V}{V_0}\right)^{-\frac{2}{3}}\left(1 - \left(\frac{V}{V_0}\right)^{\frac{1}{3}}\right)\exp\left[\left\{\frac{3}{2}(B_0' - 1)\right\}\left\{1 - \left(\frac{V}{V_0}\right)^{\frac{1}{3}}\right\}\right] \quad (2)$$

$$P_M = \frac{B_{os}}{B'_{os}}\left[\left(\frac{V}{V_0}\right)^{-B_{os}} - 1\right] \quad (3)$$

$$P_S = B_o\left[1 - \frac{V}{V_o}\right] + \frac{B_o(B_o' + 1)}{2}\left[1 - \frac{V}{V_o}\right]^2 \quad (4)$$

$$P = -\frac{\partial U}{\partial V} + P_{th} \quad (5)$$

$$P_{S-K} = B_0\left(1 - \frac{V}{V_0}\right) + \left\{\frac{B_0(B_0' + 1)}{2}\right\}\left(1 - \frac{V}{V}\right)^2 \quad (6)$$

$$P_{C-K} = B_o\left[\left(1 - \frac{V}{V_o}\right) + \frac{5}{2}\left(1 - \frac{V}{V_o}\right)^2\right] \quad (7)$$

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[5,9,10]. Therefore, it would be important to use various EOSs to formulate the change of BT under the influence of high pressure.

B_T variation with high pressure using - Birch-Murnaghan EOS

By using Eq. 1 it is found that (Eq. 9). When Eq. 9 is substituted for Eq. 8, B_T at high pressure P is obtained, which is assessed using- Birch-Murnaghan EOS provided Eq. 10. Where, $\eta=V/V_0$

B_T change with P using Vinet EOS

If Eq. 2 is used as a starting point and Eq. 8 is used to adjust for the derivative $\partial P_V/\partial V$, $(B_T)_V$ – high pressure depending on Vinet EOS is expressed by Eq. 11).

B_T change with P using Kholiya and Chandra EOS[4]

The derivative stated in Eq. 12 may be calculated from equation 7.

When Eq. 12 is substituted for Eq. 8, the resulting value is $(B_T)_{K-C}$, which represents the bulk modulus at high pressure as measured by Kholiya and Chandra. In (Eq. 13).

B_T change with P_{S-K} using (Singh and Kao) EOS [4]

$\partial P_{S-K}/\partial P$ From eq.6 the derivative presented in the following equation as (Eq. 14). From Eq. 14 and Eq. 8, we obtain Eq. 15. Where, $(B_T)_{S-K}$: bulk - modulus under high pressure evaluated according to Singh and Kao EOS.

RESULTS AND DISCUSSION

Table 1 gives the B_0 and B_0' values for C_{60}, C_{70}, C_{84}, and CNT

Compressed volume (V/V_0)

Taking into consideration the values of B_0 and B_0' form Table 1 and use them in Birch-Murnaghan and Vinet EOSs, (eqs. 1 and 2 respectively), and solving EOS (Eq. 6 and Eq. 7) we will get results of the variation of V/V_0 with pressure. These results are compared with the experimental results are shown in (Fig.1) for C_{60},C_{70},C_{84} and CNT respectively.

$$B_T = -V\left(\frac{\partial P}{\partial V}\right)_T \quad (8)$$

$$\frac{\partial P_{B-M}}{\partial V} = \frac{3B_0}{2}\left[(-\frac{7}{3})\frac{V^{-\frac{7}{3}-1}}{V_0^{-\frac{7}{3}}} + (\frac{5}{3})\frac{V^{\frac{5}{3}-1}}{V_0^{-\frac{5}{3}}} + (\frac{9}{4})(B_0' - 4)\frac{V^{-3-1}}{V_0^{-3}} - (\frac{7}{2})(B_0' - 4)\frac{V^{-\frac{7}{3}-1}}{V_0^{-\frac{7}{3}}} + \frac{5}{4}(B_0' - 4)\frac{V^{-\frac{5}{3}-1}}{V_0^{-\frac{5}{3}}}\right] \quad (9)$$

$$(B_T)_{B-M} = \frac{3B_0}{2}\left[(\frac{7}{3})\eta^{-\frac{7}{3}} - \frac{5}{3}\eta^{-\frac{5}{3}} - \frac{9}{4}(B_0' - 4)\eta^{-3} + \frac{7}{2}(B_0' - 4)\eta^{-\frac{7}{3}} - \frac{5}{4}(B_0' - 4)\eta^{-\frac{5}{3}}\right] \quad (10)$$

$$(B_T)_V = \left[2B_0(\eta^{-\frac{2}{3}} - \eta^{-\frac{1}{3}}) + B_0\eta^{-\frac{1}{3}} + \frac{3}{2}B_0(B_0' - 1)(\eta^{-\frac{1}{3}} - 1)\right]\exp\left[\left\{\frac{3}{2}(B_0' - 1)\right\}(1 - \eta^{\frac{1}{3}})\right] \quad (11)$$

$$\frac{\partial P_{K-C}}{\partial V} = -\frac{B_0}{V_0} - 5\frac{B_0}{V_0}(1 - \frac{V}{V_0}) \quad (12)$$

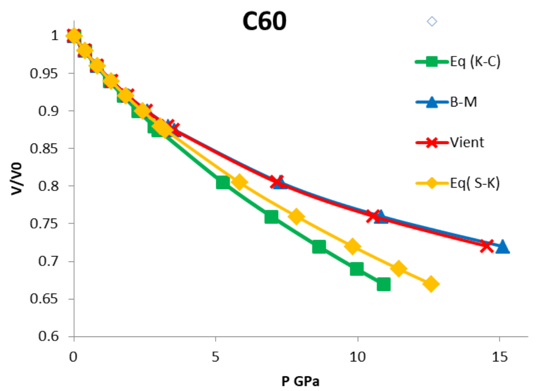
$$(B_T) = \eta B_0 + 5\eta B_0(1 - n) \quad (13)$$

$$\frac{\partial P_{S-K}}{\partial V} = -\frac{B_0}{V_0} + [B_0(B_0' + 1)(1 - \frac{V}{V_0}) * -\frac{1}{V_0}] \quad (14)$$

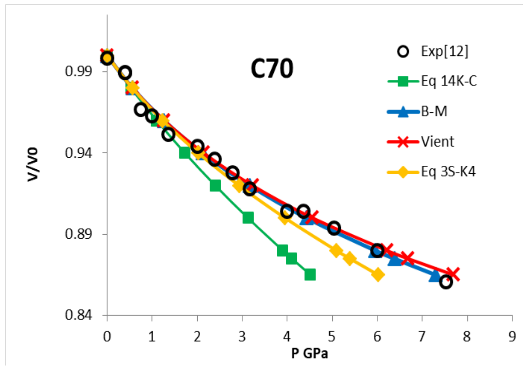
$$(B_T)_{S-K} = \eta * B_0 + (B_0 * (B'_0 + 1) * (1 - \eta) * \eta) \quad (15)$$

Table 1. B_0 and B_0' data for C_{60}, C_{70}, C_{84} and CNT.

Materials	B0 (GPa)	B'0	Ref
C_{60}	18.1	5.7	[11]
C_{70}	25	10.6	[12]
C_{84}	20	16.1	[13]
CNT individual	230	4.5	[14]
CNT Bundle	37	11	[15]



(a)



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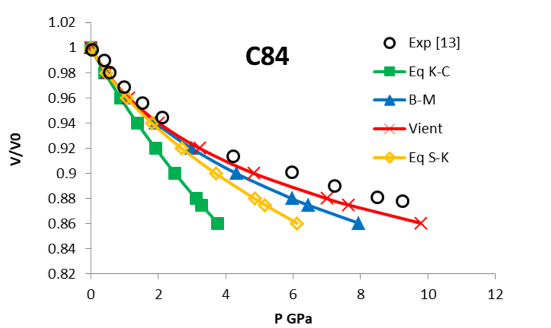

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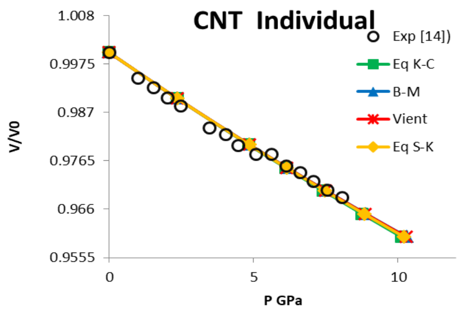

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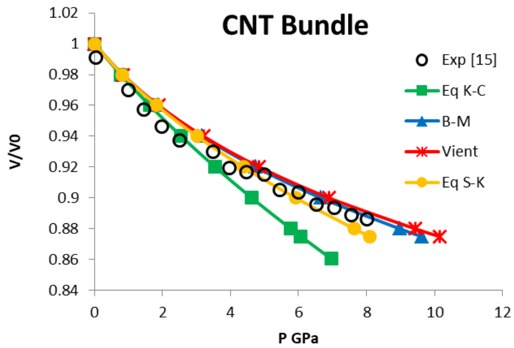

(e)

Fig. 1. Variation of V/V_0 with P for nano material C60, C70, C84 and CNT Using various EOSs compared with experimental data, using B_0, B_0' data from Table -I.

The results of Fig. 1 suggest the Vinent and Birch-Murnaghan EOSs which are derived to deal with bulk materials, may be used in the high-pressure calculations for nanomaterials.

Bulk modulus variation with P

For the nanomaterials C_{60}, C_{70}, C_{84}, and CNT, respectively, (Fig. 2) demonstrate fluctuation of B_T against high pressure. Eqs. 10, 11, 13, and 15 and B_0, B_0' values from Table-I were used to analyze these results.

From study, the V/V_o change against high pressure for nanomaterials C60, C70, C84, and CNT is calculated using four EOSs (Eqs. 1, 2, 6, and 7). The findings illustrated in Fig.1 suggest that computations for nanomaterials may be evaluated

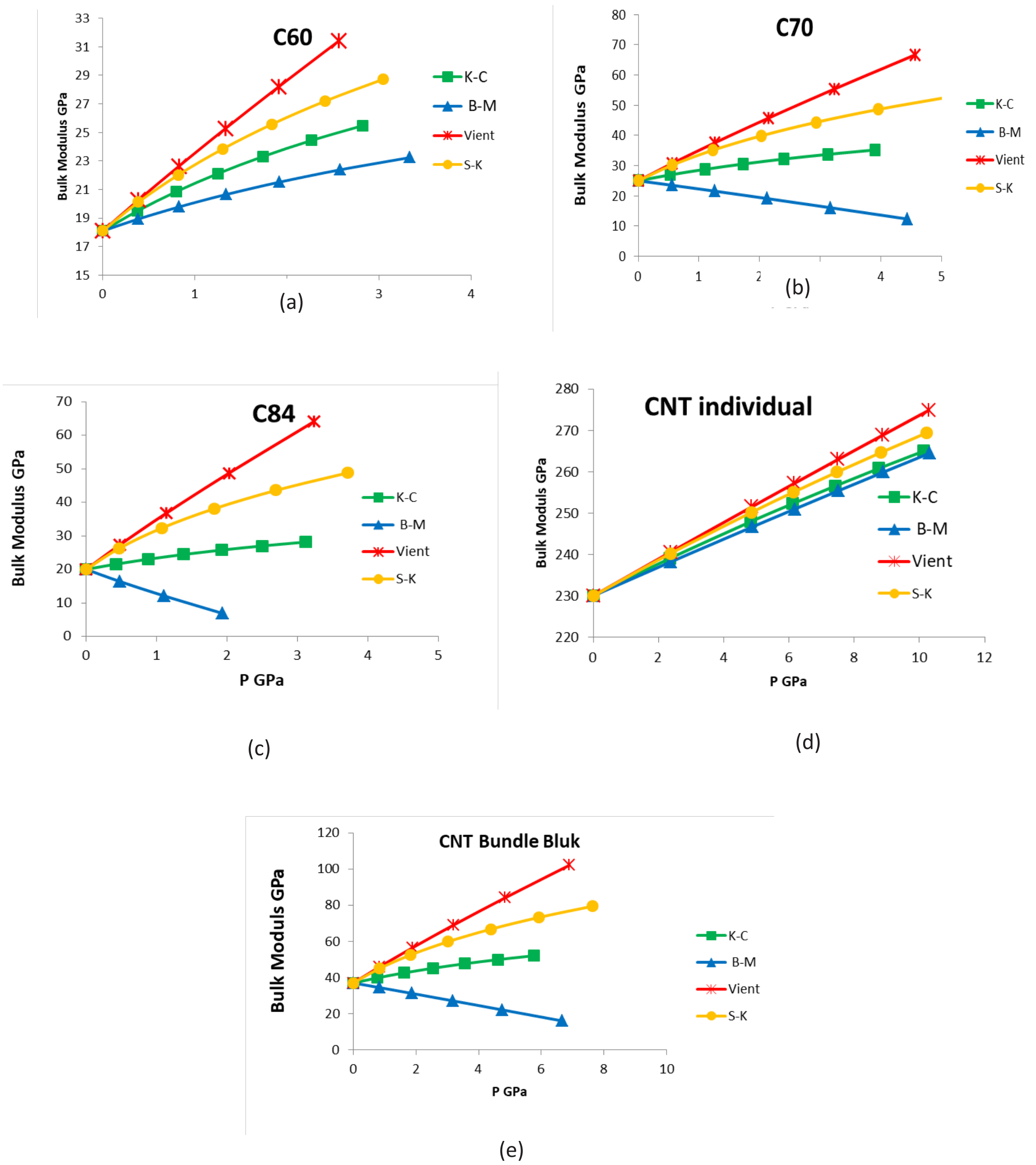

Fig. 2. Variation of B_T with P for C_{60}, C_{70}, C_{84} and CNT nano materials respectively. These results were analyzed using the equations -10, 11, 13, 15 and the B_0, B_0' values from Table 1.

using EOSs specified for bulk- materials ,such as the Birch-Murnaghan and Vinet- EOSs given in equations 1,2. Between experimental data and those computed using bulk EOSs, the findings demonstrate good agreement.

EOSs are depicted in equations- 4, 6, and 7, which were developed by the researchers [2-4] respectively constitute, in modified formalism, a single equation. Therefore, comparison of the results from equation -6, Fig. 1 with results of equation 7 show a small difference since B_o' in equation 7 has been fixed to 4. Between experimental data and those computed using nano EOSs, the findings demonstrate good agreement.

From Fig. 2 a,b,c and d the variation is due the fact that B-M EOS is derived on the basis of the macroscopic mechanical properties, while Vinet EOS is based in its derivation on the interatomic potentials. Also, the value of B_o' is fixed to 4 in the S-K and K-C EOSs.

CONCLUSION

The current work concludes that it may be possible to assess computations for nano-martials by EOSs designed for bulk- martials, such as Birch-Murnaghan and Vient EOSs. Additionally, this study suggests that the EOSs of the researchers [2-4] are essentially just one EOS, with the exception of the fact that Bo' is assumed to have a constant value of 4.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

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