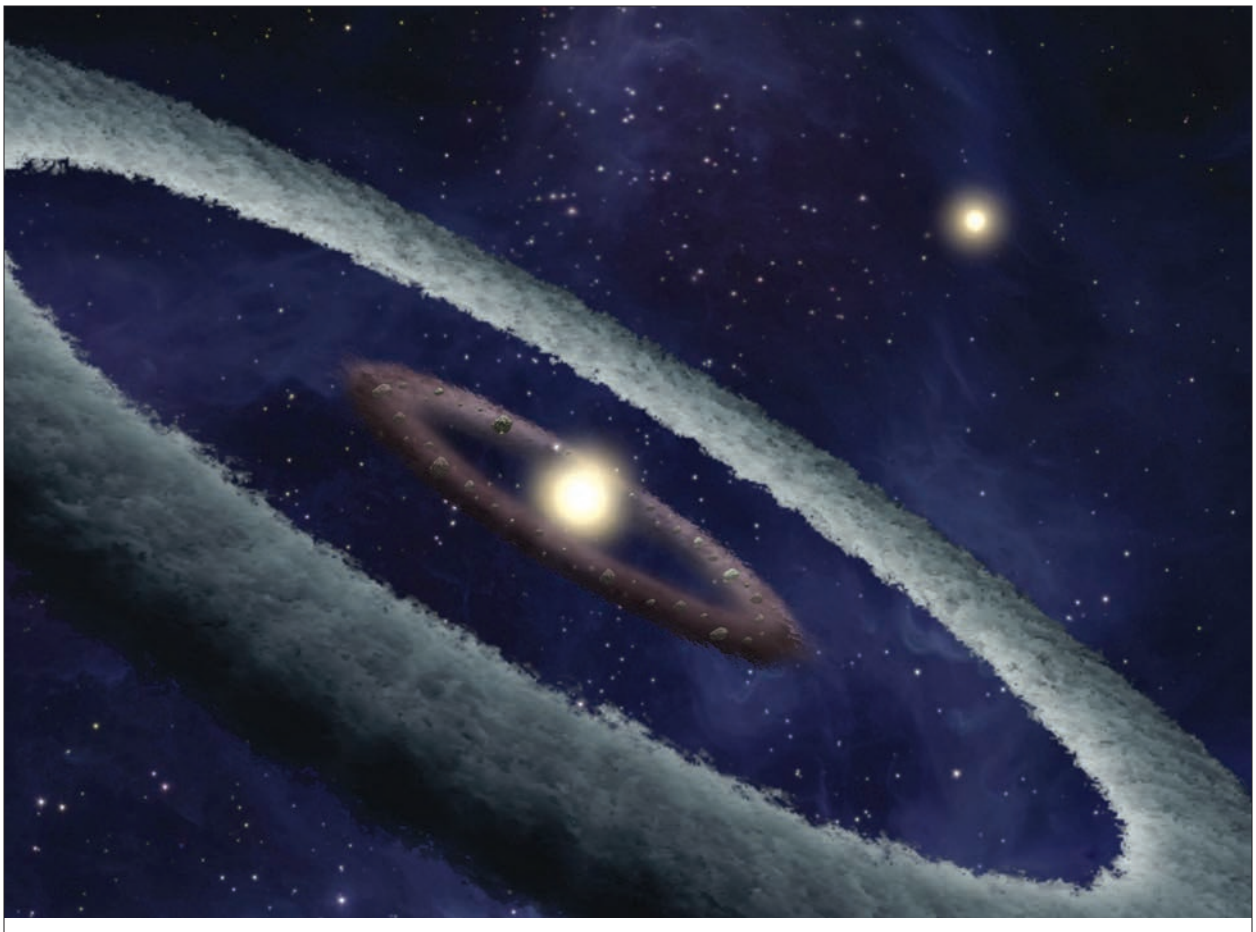

Research Journal of Physics

ISSN 1819-3463

Academic Journals Inc.

www.academicjournals.com

Research Journal of Physics 9 (1): 11-20, 2015
ISSN 1819-3463 / DOI: 10.3923/rjp.2015.11.20

Validity of High Pressure Isothermal Equation of State for Carbon Nanotubes

[1]A.K. Pandey, [2]H.K. Rai, [3]B.K. Pandey, [3]Abhay P. Srivastava and [3]C.K. Singh
[1]Department of Applied Science, Sherwood College of Engineering Research and Technology, Barabanki, Uttar Pradesh, India
[2]Solid State Chemistry Laboratory, Department of Chemistry, Sri J.N. (PG) College, Lucknow, India
[3]Department of Applied Science, MMM University of Technology, Gorakhpur, Uttar Paradesh, India

Corresponding Author: A.K. Pandey, Department of Applied Science, Sherwood College of Engineering Research and Technology, Barabanki, Uttar Paradesh, India

ABSTRACT

To predict the most suitable EOS for the analysis of real compression behavior of carbon nanotube bundles, single carbon nanotubes and Graphite we have used Suzuki, Shanker, Tait and Murnaghan Equation of states. The analysis of computed results suggests that the Suzuki formulation is not capable of explaining the compression behavior of nanomaterials at higher pressure. Shanker formulation gives slightly better results of volume compression at different pressure than the Suzuki formulation but the results obtained by Tait's and Murnaghan EOS are in good agreement to the experimental data for nanotube bundle and individual carbon nanotubes in the entire range of pressure. Surprisingly it is observed that only Murnaghan formulation gives the better agreement with the experimental results for graphite than Tait's formulation. Thus it is concluded that, the well known and widely used Murnaghan EOS is still most suitable and valid for the bulk as well as nanomaterials. The present study also reveals the fact that individual carbon nanotubes are less compressible than bundles of carbon nanotubes.

Key words: Equation of state, high pressure, compression behaviour, carbon nanotubes, graphite, bulk modulus, pressure derivative of bulk modulus

INTRODUCTION

Carbon nanotubes (Iijima, 1991) got a lot of attention due to their potential uses in the devices exploiting their unusual mechanical and electronic properties. The elastic behavior of carbon nanotubes to the external force or stress are very important due to their excellent applications in the engineering, industry and medical field (Dresselhaus *et al*., 1996; Vigolo *et al*., 2000).

When one sheet or multiple sheets of graphene rolled into a cylinder gives a one-dimensional structure of carbon nanotubes. Single-walled carbon nanotube bundles typically consist of several nested tubes, each like a graphene sheet bent into the cylindrical form with an overall diameter of a few nanometers. Single-walled carbon nanotubes can be classified according to different chiral angles, for example zigzag ($\theta = 0°$), armchair ($\theta = 30°$) and chiral tubes ($0°<\theta<30°$) (Dresselhaus *et al*., 1995). The elastic properties such as Young's modulus and Poisson's ratio of nanotube have been studied by the previous workers (Lu, 1997a; Hernandez *et al*., 1999; Sanchez-Portal *et al*., 1999; Van Lier *et al*., 2000). The hardness and its important relation with mechanical properties of single-walled carbon nanotubes have been intensively studied during the last decade (Lu, 1997b; Hernandez *et al*., 1999; Sanchez-Portal *et al*., 1999; Van Lier *et al*., 2000; Yakobson *et al*., 1996).

Grain-size and grain-shape parameters have a great influence on the physical properties of materials and on geophysical processes. With the decrease of grain size, the deformation mechanism passes from dislocation-controlled creep to diffusion-controlled creep.

Physical properties of earth materials deep down the earth are usually studied at micro or millimetric scales but not at nanometric scale. Even though nanocrystalline material might have an important influence on geological processes (Hochella *et al*., 2008), they are very poorly studied. High pressures which are encountered from deep down the earth to the astrophysical objects may cause many effects such as compression, pressure ionization, modification in electronic properties, phase changes and several phenomenon in applied fields (Schilling, 1998).

Usually the study of pressure versus volume relations of condensed matter is done by equation of states. There are many equations of state described in the literature but still there is severe need to search a simple and most suitability equation of state which is applicable in the entire range of compressions. It is observed that the most of EOS give the same result under small compression. The classical theory of infinitesimal elasticity is based on two assumptions:

- The strain is uniquely determined by the stresses and are reversible
- The strain are limited to 'linear elasticity', that is they are so small that the squares and products are negligible

In the finite strain, the first assumption is retained but the restriction to small strain is removed (Murnaghan, 1937). In generalized elasticity theory, finite strain representations but practical expressions for finite strain were developed by Birch (1952). He used Murnaghan's basic theory but restricted it to the case where the initial stress is a large hydrostatic pressure. The crucial assumption in finite strain theory is the formal relationship between compression and coordinate displacement (Stacey *et al*., 1981). For the analysis of compression behavior at high pressure, generally the finite strain theory proposed by Birch is used (Birch, 1952). The attention has also been given to the theory based on atomic potential as presented by Rydberg (1932). On the basis of The Mie Gr¨uneisen theory Suzuki proposed formulation to analysis the high compression behavior of materials (Suzuki *et al*., 1979; Anderson, 1995; Helffrich, 1999). The Gr¨uneisen theory of thermal expansion as formulated by Born and Huang (1995) has been used by Shanker *et al*. (1997a). These authors included a higher order term for the change in the expansion of potential energy. Using some thermodynamical relation Tait formulated a relation (Shanker *et al*., 1997b; Murnaghan, 1944; Taravillo *et al*., 2002) known as Tait equation of state. The well known and widely used EOS (Murnaghan, 1944) is the Murnaghan EOS which is based on the assumption that the isothermal bulk modulus is the linear function of pressure at any particular temperature.

In the present study, we have studied the mechanical properties especially volume compression (V/V_0) of nanotube bundles, individual carbon nanotubes and graphite using widely used Suzuki, Shanker, Tait and Murnaghan Equation of State (EOS) (Stacey *et al*., 1981; Rydberg, 1932; Suzuki *et al*., 1979; Anderson, 1995; Helffrich, 1999; Born and Huang, 1995; Shanker *et al*., 1997a; Murnaghan, 1944; Taravillo *et al*., 2002; Singh *et al*., 2001; Kandpal *et al*., 2004). Calculated results are compared with the experimental values. It is observed that, Murnaghan formulation gives the almost same results as reported by Chandra *et al*. (2013) calculated by using usual Tait's equation for the bundles of carbon nanotubes and individual carbon nanotubes. In case of graphite it is

observed that the computed results for graphite using Murnaghan EOS have better agreement with experimental results than reported results computed by Chandra *et al*. (2013) using usual Tait's equation of state.

For input parameters the values of bulk modulus and its first order pressure derivative for carbon nanotube bundles and individual tube within the bundle are taken from Reich *et al*. (2002). The input values of bulk modulus K_T and its first order pressure derivative for graphite K_T' are taken from Hanfland *et al*. (1989).

The K_0 = 37 GPa, K'_0 = 11 and individual tube within the bundle (K_0 = 230 GPa, K'_0 = 4.5) have been taken from the work of Reich *et al*. (2002). They have calculated these values using local-density approximation of density-functional theory. The values of bulk modulus and its first order pressure derivative for graphite are taken to be K_0 = 33.8 GPa and K'_0 = 8.9, as measured by Hanfland *et al*. (1989) from X-ray diffraction studies.

MATERIALS AND METHODS

Taits EOS: The oldest EOS is called Tait EOS or linear elastic modulus equation (Hayward, 1967; Borelius, 1958) which was formulated as:

$$\frac{V}{V_0} = 1 - \frac{aP}{b + P} \tag{1}$$

With:

$$a = \frac{2}{K_0^{'} + 1}$$

and:

$$b = \frac{2K_0}{K_0^{'} + 1}$$

another EOS given by Tait is:

$$\frac{V}{V_0} = 1 - a\log(1 + bP) \tag{2}$$

With:

$$a = \frac{1}{K_0^{'} + 1}$$

and:

$$b = \frac{K_0^{'} + 1}{K_0}$$

The simplest form of Tait'S EOS for compression and bulk modulus can be expressed as (Devlal and Kholiya, 2006):

$$\frac{V}{V_0}=\left[1-\frac{1}{K_0^{'}+1}\log\left\{1+\left(\frac{K_0^{'}+1}{K_0}\right)P\right\}\right] \tag{3}$$

This is Tait EOS.

Murnaghan EOS: The well known and widely used EOS (Murnaghan, 1944) is the Murnaghan EOS which is based on the assumption that isothermal bulk modulus K is linear function of pressure at any temperature that is:

$$K(P, T) = K_0+K'_0P \tag{4}$$

Using the definition of bulk modulus and integrating Eq. 4 at constant temperature we get the Murnaghan EOS as follows:

$$\frac{V}{V_0}=\left(1+\frac{K_0^{'}}{K_0}P\right)^{\frac{-1}{K_0^{'}}} \tag{5}$$

This is Muenaghan EOS.

Shanker EOS: The Gruneisen theory of thermal expansion as formulated by Born and Huang (1995) has been used by Shanker *et al*. (1997b). These authors included higher order term for the change in volume in the expansion of potential energy and claimed to derive a new expression for V/V_0 which is given by:

$$\frac{V}{V_0}-1=\frac{1-\left[1-2\left\{\left(K_0^{'}+1\right)/K_0\right\}P_{Th}\right]^{1/2}}{\left(K_0^{'}+1\right)} \tag{6}$$

It has been argued by Kushwaha and Shanker (1998) that the above EOS may be written as:

$$\frac{V}{V_0}-1=\frac{1-\left[1-2\left\{\left(K_0^{'}+1\right)/K_0\right\}(P-P_{Th})\right]^{1/2}}{\left(K_0^{'}+1\right)} \tag{7}$$

When thermal pressure is zero ($P_{Th} = 0$) then above equation becomes:

$$\frac{V}{V_0}=\frac{1-\left[1+2\left\{\left(K_0^{'}+1\right)/K_0\right\}P\right]^{1/2}}{\left(K_0^{'}+1\right)}+1 \tag{8}$$

This is Shanker EOS.

Suzuki EOS: San-Miguel and Suzuki (San-Miguel, 2006; Suzuki, 1975) have followed the Gruneisen theory of thermal expansion based on the Mie Gruneisen equation of state (Anderson, 1995):

$$PV+X(V) = \gamma E_{Th} \tag{9}$$

where, P is pressure, X(V) = dφ/dV, φ is potential energy as a function of volume only, γ is the Gruneisen parameter regarded as constant and E_{Th} is the thermal energy of lattice vibration. After using Taylor's expansion in the second term of Eq. 9 we get the equation:

$$\frac{V}{V_0} = \frac{\left[1+2k-\left\{1-\left(4kE_{Th}/Q\right)\right\}^{1/2}\right]}{2k} \tag{10}$$

In the Mie-Gruneisen EOS:

$$P_{Th} = \frac{\gamma E_{Th}}{V_0}$$

and:

$$Q = \frac{K_0 V_0}{\gamma}$$

Substituting the value P_{Th} in Eq. 10 we get:

$$\frac{V}{V_0} = \frac{1+2k-\left\{1-\left(4kP_{Th}V/K_0V_0\right)\right\}^{1/2}}{2k} \tag{11}$$

Taking:

$$k = \frac{K_0^{'}-1}{2}$$

where, K'_0 is first pressure derivative of isothermal bulk modulus at 0 pressure, we get:

$$\frac{V}{V_0} = \frac{1+\left(K_0^{'}-1\right)-\left[1-2\left\{\left(K_0^{'}-1\right)/K_0\right\}P_{Th}\right]^{1/2}}{\left(K_0^{'}-1\right)} \tag{12}$$

where, P_{Th} is thermal pressure. If pressure P is not equal to zero then Eq. 12 written as:

$$\frac{V}{V_0} = \frac{1+\left(K_0^{'}-1\right)-\left[1-2\left\{\left(K_0^{'}-1\right)/K_0\right\}\left(P_{Th}-P\right)\right]^{1/2}}{\left(K_0^{'}-1\right)}$$

When thermal pressure P_{Th} is equal to zero then above equation becomes:

$$\frac{V}{V_0} = \frac{1-\left[1+2\left\{\left(K_0^{'}-1\right)/K_0\right\}P\right]^{1/2}}{\left(K_0^{'}-1\right)}+1 \quad (13)$$

This is Suzuki EOS.

RESULTS AND DISCUSSION

In the present study, we have taken four widely used different EOS based on inter atomic potential model and strain theory model viz., Tait, Murnaghan, Shanker and Suzuki to study the volume compression (V/V_0) of nanotube bundles, individual carbon nanotubes and graphite. The values of volume compression (V/V_0) at different pressure have been calculated by using Eq. 3, 5, 8 and 13 for carbon nanotube bundles, individual carbon nanotubes and graphite. The input values of K_0 (GPa) and K_0' for carbon nanotube bundles, individual carbon nanotubes and graphite are taken from Reich *et al*. (2002) and Hanfland *et al*. (1989) as mentioned in the Table 1. We have presented the calculated values of volume compression with pressure for carbon nanotube bundles and individual carbon nanotubes using different equation of states viz., Suzuki, Shanker, Tait and Murnaghan Equation of State (EOS) in the Table 2 and 3, respectively. The values of volume compression with pressure (GPa) for graphite have been given in Table 4. Graphical representation of computed values of volume compression at different pressure using different EOS for carbon nanotube bundles and individual carbon nanotubes and graphite are shown in Fig. 1a-c, respectively. Our main objective is to analyze the validity of most suitable and simple equation of state for nanomaterials as well as bulk materials. In our present study we have considered graphite

Table 1: Input parameters K_0 (GPa) and K_0' for carbon nanotube bundles, individual carbon nanotubes and graphite

Materials	K_0 (GPa)	K_0'	References
Carbon nanotube bundles	37.0	11.0	Reich *et al*. (2002)
Individual carbon nanotubes	230.0	4.5	Reich *et al*. (2002)
Graphite	33.8	8.9	Hanfland *et al*. (1989)

Table 2: Calculated values of volume compression at different pressure for carbon nanotube bundles and individual carbon nanotubes using Tait equation of states (Eq. 3), Murnaghan EOS (Eq. 5), Shanker EOS (Eq. 8) and Suzuki EOS (Eq. 13) along with experimental value (Reich *et al*., 2002)

P (GPa)	V/V_0 (Eq. 3)	V/V_0 (Eq. 5)	V/V_0 (Eq. 8)	V/V_0 (Eq. 13)	V/V_0 Exp. Reich *et al*. (2002)	Dev. (%) (Eq. 3)	Dev. (%) (Eq. 5)	Dev. (%) (Eq. 8)	Dev. (%) (Eq. 13)
1.0	0.9766	0.9766	0.9763	0.9759	0.9769	0.030709	0.030709	0.061419	0.102365
1.5	0.9670	0.9670	0.9663	0.9654	0.9638	0.332019	0.332019	0.259390	0.166010
2.0	0.9583	0.9585	0.9570	0.9557	0.9513	0.735835	0.756859	0.599180	0.462525
2.5	0.9505	0.9507	0.9484	0.9467	0.9425	0.848806	0.870027	0.625995	0.445623
3.0	0.9434	0.9437	0.9403	0.9381	0.9400	0.361702	0.393617	0.031915	0.202128
3.5	0.9368	0.9372	0.9326	0.9299	0.9350	0.192513	0.235294	0.256684	0.545455
4.0	0.9307	0.9312	0.9253	0.9222	0.9238	0.746915	0.801039	0.162373	0.173198
4.5	0.9250	0.9257	0.9184	0.9147	0.9213	0.401606	0.477586	0.314773	0.716379
5.0	0.9197	0.9205	0.9117	0.9076	0.9188	0.097954	0.185024	0.772747	1.218981
5.5	0.9147	0.9157	0.9052	0.9007	0.9088	0.649208	0.759243	0.396127	0.891285
6.0	0.9100	0.9111	0.8990	0.8940	0.9063	0.408253	0.529626	0.805473	1.357167
6.5	0.9055	0.9068	0.8930	0.8875	0.8981	0.823962	0.968712	0.567865	1.180269
7.0	0.9013	0.9028	0.8872	0.8813	0.8963	0.557849	0.725204	1.015285	1.673547
7.5	0.8972	0.8989	0.8815	0.8752	0.8900	0.808989	1	0.955056	1.662921
8.0	0.8934	0.8952	0.8760	0.8693	0.8875	0.664789	0.867606	1.295775	2.050704

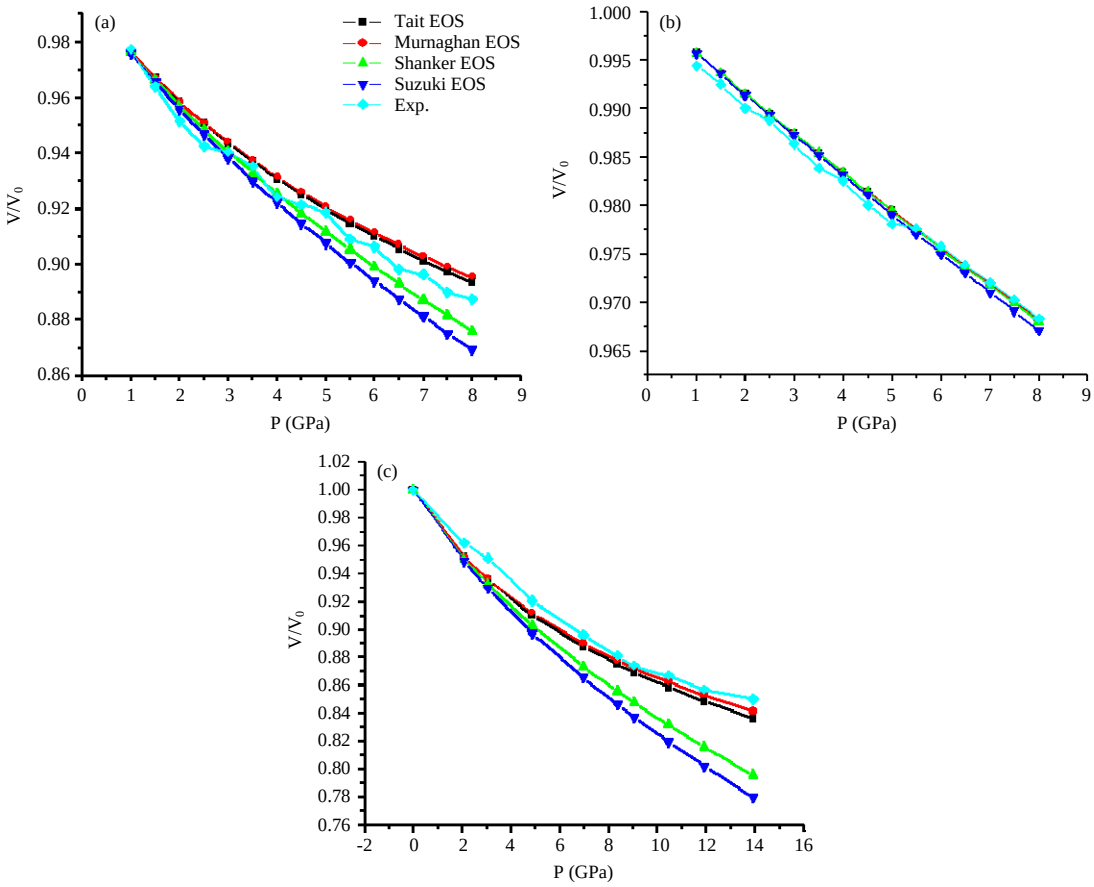

Fig. 1(a-c): Compression behavior of (a) Carbon nanotube (bundles), (b) Carbon nanotube (individual) and (c) Graphite

Table 3: Calculated values of volume compression at different pressure for individual carbon nanotubes using Tait equation of states (Eq. 3), Murnaghan EOS (Eq. 5), Shanker EOS (Eq. 8) and Suzuki EOS (Eq. 13) along with experimental value (Reich *et al*., 2002)

P (GPa)	V/V_0 (Eq. 3)	V/V_0 (Eq. 5)	V/V_0 (Eq. 8)	V/V_0 (Eq. 13)	V/V_0 Exp. Reich *et al*. (2002)	Dev. (%) (Eq. 3)	Dev. (%) (Eq. 5)	Dev. (%) (Eq. 8)	Dev. (%) (Eq. 13)
1.0	0.9957	0.9957	0.9957	0.9957	0.9944	0.130732	0.130732	0.130732	0.130732
1.5	0.9936	0.9936	0.9936	0.9936	0.9925	0.110831	0.110831	0.110831	0.110831
2.0	0.9915	0.9915	0.9915	0.9914	0.9900	0.151515	0.151515	0.151515	0.141414
2.5	0.9894	0.9894	0.9894	0.9893	0.9888	0.060680	0.060680	0.060680	0.050566
3.0	0.9874	0.9874	0.9874	0.9872	0.9863	0.111528	0.111528	0.111528	0.091250
3.5	0.9854	0.9854	0.9854	0.9852	0.9838	0.162635	0.162635	0.162635	0.142305
4.0	0.9834	0.9834	0.9834	0.9831	0.9825	0.091603	0.091603	0.091603	0.061069
4.5	0.9814	0.9814	0.9814	0.9811	0.9800	0.142857	0.142857	0.142857	0.112245
5.0	0.9795	0.9795	0.9794	0.9790	0.9781	0.143135	0.143135	0.132911	0.092015
5.5	0.9775	0.9775	0.9775	0.9770	0.9776	0.010229	0.010229	0.010229	0.061375
6.0	0.9756	0.9756	0.9754	0.9750	0.9757	0.010249	0.010249	0.030747	0.071743
6.5	0.9737	0.9737	0.9736	0.9730	0.9738	0.010269	0.010269	0.020538	0.082152
7.0	0.9719	0.9719	0.9718	0.9710	0.9720	0.010288	0.010288	0.020576	0.102881
7.5	0.9700	0.9700	0.9699	0.9691	0.9702	0.020614	0.020614	0.030921	0.113379
8.0	0.9682	0.9682	0.9680	0.9671	0.9683	0.010327	0.010327	0.030982	0.123929

as bulk material. The analysis of computed results of volume compression at different pressure from P = 1-8.00 GPa obtained from Suzuki formulation shows that it do not agree with the

Table 4: Calculated values of volume compression at different pressure for graphite using Tait equation of states (Eq. 3), Murnaghan EOS (Eq. 5), Shanker EOS (Eq. 8) and Suzuki EOS (Eq. 13) along with experimental value (Reich *et al*., 2002)

P (GPa)	V/V_0 (Eq. 3)	V/V_0 (Eq. 5)	V/V_0 (Eq. 8)	V/V_0 (Eq. 13)	V/V_0 Exp. Reich *et al*. (2002)	Dev. (%) (Eq. 3)	Dev. (%) (Eq. 5)	Dev. (%) (Eq. 8)	Dev. (%) (Eq. 13)
0	1	1	1	1	1	0	0	0	0
2.087	0.9518	0.9520	0.9504	0.9487	0.9618	1.039717	1.018923	1.185278	1.362030
3.0434	0.9356	0.9360	0.9325	0.9296	0.9507	1.588303	1.546229	1.914379	2.219417
4.8696	0.9105	0.9115	0.9027	0.8975	0.9204	1.075619	0.966971	1.923077	2.488049
6.9565	0.8878	0.8896	0.8735	0.8656	0.8961	0.926236	0.725365	2.522040	3.403638
8.3478	0.8751	0.8775	0.8559	0.8463	0.8809	0.658418	0.385969	2.838007	3.927801
9.0434	0.8693	0.8721	0.8475	0.8372	0.8737	0.503605	0.183129	2.998741	4.177635
10.434	0.8586	0.8621	0.8316	0.8197	0.8665	0.911714	0.507790	4.027698	5.401039
11.913	0.8483	0.8525	0.8157	0.8022	0.8566	0.968947	0.478636	4.774691	6.350689
13.913	0.8359	0.8411	0.7955	0.7798	0.8500	1.658824	1.047059	6.411765	8.258824

experimental data (Reich *et al*., 2002; Hanfland *et al*., 1989) at higher pressure ranges while Shanker formulation gives slightly better results than Suzuki, however, all the said EOS are giving similar results at low pressure. Same conclusion has also been made by Chandra *et al*. (2013). Failure of Suzuki and Shanker formulation may be attributed to the fact that their formulation is based on approximation. The Suzuki formulation is based on the Taylor series expansion of potential energy, in which higher order terms beyond second order have been neglected. This approximation must introduce serious errors as discussed in detail by Wang and Reeber (1998). Similar to the Suzuki model, Shanker *et al*. (1997b) have also neglected higher order terms in deriving Eq. 8.

The results obtained by Tait's EOS is in good agreement with experimental results especially for carbon nanotube bundles and individual carbon nanotubes for the entire range of pressure having maximum deviation upto <1% with experimental values of volume compression as it is also reported by Chandra *et al*. (2013) but when this EOS is tested for bulk sample of graphite it deviates upto 1.65% from the experimental results (Reich *et al*., 2002; Hanfland *et al*., 1989) for calculation of volume compression at pressure ranges 0-13.91 GPa. Due to unavailability of experimental data above 13.91 GPa the further comparison is not be possible. The results obtained by Murnaghan EOS are not only very close to the experimental results for carbon nanotube bundles and individual carbon nanotubes but also for the graphite. It is also observed that the results obtained for graphite is in better agreement than the results obtained by Tait's formulation for the entire range of pressure.

The validity of Tait's formulation for carbon nanotube bundles and individual carbon nanotubes can be justified on the basis of the fact that the product of bulk modules and the coefficient of volume thermal expansion remain constant for carbon nanotubes but it is not applicable for bulk materials like graphite, due this reason the results of Tait's formulation deviates in case of graphite. On the other hand, the validity of Murnaghan formulation can be justified on the basis of the fact that isothermal bulk modulus K is linear function of pressure at any temperature for bulk as well as nanomaterials. When more number of carbon nanotubes in a bundle is examined by Munaghan formulation then it may deviate slightly but its use for individual carbon nanotubes and bulk material will be better that Tait's formulation. Thus we conclude that the well known and widely used Murnaghan EOS (Murnaghan, 1944) is still most suitable and valid for the bulk as well as nanomaterials.

CONCLUSION

The analysis of results obtained in the present study may be concluded that the Suzuki formulation fails to explain the high pressure compression behavior of carbon nanotubes, Shanker formulation slightly improves the result of Suzuki formulation but not upto the mark. Tait's

formulation is suitable to explain the high pressure compression behavior of carbon nanotube bundles and individual carbon nanotubes but its result deviates from the experimental results in case of bulk materials. On the other hand, the results obtained by Murnaghan EOS are not only very close to the experimental results for carbon nanotube bundles and individual carbon nanotubes but also for graphite during the entire range of pressure. Thus we conclude that the well known and widely used Murnaghan EOS is still most suitable and valid for the bulk as well as nanomaterials for theoretical prediction of volume compression at extreme pressure where the experimental determination is not possible.

REFERENCES

Anderson, O.L., 1995. Equation of State for Geophysics and Ceramic Science. Oxford University Press, Oxford, UK., Pages: 405.

Birch, F., 1952. Elasticity and constitution of the Earth's interior. J. Geophys. Res., 57: 227-286.

Borelius, G., 1958. Changes of State of Simple Solid and Liquid Metals. Seitz, F. and D. Turnbull (Eds.). Solid State Physics: Advances in Research and Applications, Academic Press, New York, USA.,-pp: 65-94.

Born, M. and K. Huang, 1995. Dynamical Theory of Crystal Lattice. Oxford University Press, Oxford, UK.

Chandra, J., P.K. Bhatt and K. Kholiya, 2013. Analysis of equation of state for carbon nanotubes. J. Nanotechnol. 10.1155/2013/639068

Devlal, K. and K. Kholiya, 2006. Analysis of equations of state for metals and rare gas solids. Ind. J. Phys., 80: 801-805.

Dresselhaus, M.S., G. Dresselhaus and R. Saito, 1995. Physics of carbon nanotubes. Carbon, 33: 883-891.

Dresselhaus, M.S., G. Dresselhaus and P.C. Eklund, 1996. Science of Fullerenes and Carbon Nanotubes. Academic Press, San Diego, USA, ISBN: 9780122218200, Pages: 965.

Hanfland, M., H. Beister and K. Syassen, 1989. Graphite under pressure: Equation of state and first-order Raman modes. Phys. Rev. B, Vol. 39. 10.1103/PhysRevB.39.12598

Hayward, A.T.J., 1967. Compressibility equations for liquids: A comparative study. Br. J. Applied Phys., 18: 965-965.

Helffrich, G., 1999. Practical use of Suzuki's thermal expansivity formulation. Phys. Earth Planetary Inter., 116: 133-136.

Hernandez, E., C. Goze, P. Bernier and A. Rubio, 1999. Elastic properties of single-wall nanotubes. Applied Phys. A, 68: 287-292.

Hochella, M.F., S.K. Lower, P.A. Maurice, R.L. Penn, N. Sahai, D.L. Sparks and B.S. Twining, 2008. Nanominerals, mineral nanoparticles and earth systems. Science, 319: 1631-1635.

Iijima, S., 1991. Helical microtubules of graphitic carbon. Nature, 354: 56-58.

Kandpal, D., K.Y. Singh and B.R.K. Gupta, 2004. On pressure dependence of the relative compression (V/V_0) at room temperature for the solids: Copper and lead as prototypes. Ind. J. Phys. A, 78: 393-395.

Kushwah, S.S. and J. Shanker, 1998. On the temperature dependence of thermal expansivity of NaCl crystal. Indian J. Pure Applied Phys., 36: 46-48.

Lu, J.P., 1997a. Elastic properties of carbon nanotubes and nanoropes. Phys. Rev. Lett., Vol. 79, No. 7. 10.1103/PhysRevLett.79.1297

Lu, J.P., 1997b. Elastic properties of single and multilayered nanotubes. J. Phys. Chem. Solids, 58: 1649-1652.

Murnaghan, F.D., 1937. Finite deformations of an elastic solid. Am. J. Math., 59: 235-260.

Murnaghan, F.D., 1944. The compressibility of media under extreme pressures. Proc. Natl. Acad. Sci. USA., 30: 244-251.

Reich, S., J. Maultzsch, C. Thomsen and P. Ordejon, 2002. Tight-binding description of graphene. Phys. Rev. B, Vol. 66, No. 3. 10.1103/PhysRevB.66.035412

Rydberg, R., 1932. Graphische darstellung einiger bandenspektroskopischer ergebnisse. Zeitschrift Physik, 73: 376-385.

San-Miguel, A., 2006. Nanomaterials under high-pressure. Chem. Soc. Rev., 35: 876-889.

Sanchez-Portal, D., E. Artacho, J.M. Soler, A. Rubio and P. Ordejon, 1999. *Ab initio* structural, elastic and vibrational properties of carbon nanotubes. Phys. Rev. B, Vol. 59, No. 19. 10.1103/PhysRevB.59.12678

Schilling, J.S., 1998. The use of high pressure in basic and materials science. J. Phys. Chem. Solids, 59: 553-568.

Shanker, J., B. Singh and S.S. Kushwah, 1997a. On the high-pressure equation of state for solids. Phys. B: Condensed Matter, 229: 419-420.

Shanker, J., S.S. Kushwah and P. Kumar, 1997b. Theory of thermal expansivity and bulk modulus for MgO and other minerals at high temperatures. Phys. B: Condensed Matter, 233: 78-83.

Singh, M., P.P. Singh, B.R. Gupta and M. Kumar, 2001. Temperature and pressure dependence of elastic constants. High Temp., 33: 199-206.

Stacey, F.D., B.J. Brennan and R.D. Irvine, 1981. Finite strain theories and comparisons with seismological data. Geophys. Surveys, 4: 189-232.

Suzuki, I., 1975. Thermal expansion of periclase and olivine and their anharmonic properties. J. Phys. Earth, 23: 145-159.

Suzuki, I., S.I. Okajima and K. Seya, 1979. Thermal expansion of single-crystal manganosite. J. Phys. Earth, 27: 63-69.

Taravillo, M., V.G. Baonza, J.E. Rubio, J. Nunez and M. Caceres, 2002. The temperature dependence of the equation of state at high pressures revisited: A universal model for solids. J. Phys. Chem. Solids, 63: 1705-1715.

Van Lier, G., C. van Alsenoy, V. van Doren and P. Geerlings, 2000. Ab initio study of the elastic properties of single-walled carbon nanotubes and graphene. Chem. Phys. Lett., 326: 181-185.

Vigolo, B., A. Penicaud, C. Coulon, C. Sauder and R. Pailler *et al*., 2000. Macroscopic fibers and ribbons of oriented carbon nanotubes. Science, 290: 1331-1334.

Wang, K. and R.R. Reeber, 1998. The role of defects on thermophysical properties: Thermal expansion of V, Nb, Ta, Mo and W. Mater. Sci. Eng. R: Rep., 23: 101-137.

Yakobson, B.I., C.J. Brabec and J. Bernholc, 1996. Nanomechanics of carbon tubes: Instabilities beyond linear response. Phys. Rev. Lett., Vol. 76, No. 14. 10.1103/PhysRevLett.76.2511 /PhysRevLett.76.2511