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Analytical Study of Nanomaterials under High Pressure

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Abstract

Our previous study we extended an equation of state model for second order bulk modulus from recent predicted model and calculated variation of pressure with volume for several nanomaterials. Now we use such a model for few other nanomaterials like, TiO_2 (anatase), Ni (20 nm), CdSe (rock salt phase), AlN (Hexagonal), 3C-SiC (30 nm) and Rb_3 C_{60}., compare with some other equation of state for nanomaterials and experimental data. The Microsoft Office software has been used to do the calculations. The studies gives great agreement with other EOS and experimental data. The study must be useful at high pressure when the experimental data are not available. So the given study must we useful at high pressure.

Article History

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Keywords

Bulk Modulus;
Equation of State;
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Introduction

Recently the study of nanomaterials are achieving more attention due to its surprising properties such as size, shape, morphology, compressible properties, and their structural properties changed with pressure, volume, and temperature.[1,2] So its extraordinary properties mechanical, thermal and electronic properties make it more relievable for developing several multi functional applications.[3] Synthesized and electro chemicalanodizations experimental were studied under high pressure up to 31 GPa for Anatase titanium dioxide (TiO_2) nanotubes by Raman spectroscopy and synchrotron X-ray diffraction[4] and study of a synchrotron X-ray diffraction presented pressure-induced changes innanocrystalline anatase (30-40 nm) to 35 GPa.[5]

A simple theory predicts for several nanomaterials on the effect of pressure for volume expansion[6] and high-pressure behavior of Ni-filled and Fe-filled MWCNTs examined up to 27 GPa and 19 GPa with help of synchrotron-based angle-

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dispersive X-ray diffraction.[7] A equation of state studied for several namomaterials such as metals Ni (20 nm), α-Fe (nanotubes), Cu (80 nm) and Ag (55nm), semiconductors Ge (49 nm), Si, CdSe (rock-salt phase), MgO (20 nm) and ZnO, and carbon nanotube (CNT) in term pressure related with volume and their theoretical data agreement between experimental data.[8] Plasma Enhanced Chemical Vapor Deposition (PECVD) and annealing technique are used in Crystal size synthesized of nanocrystal 3C-SiC (than 30 nm).[9] H.A. Ludwig , investigated X-ray experiments under high pressure up to 6 GPa at 300°Kfor Rb3C60using a diamond anvil cell and angular dispersive X-ray scattering.[10]

Method of Analysis

These equations of state (EOS) are determining the effect of pressure on nanomaterials, where P is a function of relative change in Volume (V/V_0) as several equations of states (EOS) written as follows: Rohit Gupta EOS written as,[11]

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$$P = B_0\left(1-\frac{V}{V_0}\right) + B_0\left\{\frac{(B_0'+1)}{2}\right\}\left(1-\frac{V}{V_0}\right)^2 + B_0\left\{\frac{(B_0B_0''+3B_0'+2)}{6}\right\}\left(1-\frac{V}{V_0}\right)^3 \quad ...(1)$$

Mie–Gruneisen EOS written as,[12]

$$P = B_0\left(1-\frac{V}{V_0}\right) + \frac{B_0(B_0'+1)}{2}\left(1-\frac{V}{V_0}\right)^2 \quad ...(2)$$

Tait EOS written as,[13]

$$P = \frac{B_0}{(B_0'+1)}\left[exp\left\{(B_0'+1)\left(1-\frac{V}{V_0}\right)\right\}-1\right] \quad ...(3)$$

Murnaghan EOS written as,[14]

$$P = \frac{B_0}{B_0'}\left[\exp\left\{-B_0'\ln\frac{V}{V_0}\right\}-1\right] \quad ...(4)$$

Birch–Murnaghan EOS written as,[15]

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

Vinet EOS written as,[16]

$$P = 3B_0\left(\frac{V}{V_0}\right)^{-2/3}\left[1-\left(\frac{V}{V_0}\right)^{1/3}\right] \times exp\left[\frac{3(B_0'-1)}{2}\left\{1-\left(\frac{V}{V_0}\right)^{1/3}\right\}\right] \quad ...(6)$$

Kholiya and Chandra EOS written as,[17]

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

Kalita and Mariotto *et al.*[24] examined experimental data for several nanomaterial compounds but here our interest only few material such as, TiO_2 (anatase), Ni (20 nm), CdSe (rock salt phase), AlN (Hexagonal), 3C-SiC (30 nm) and Rb_3C_{60}. The given experimental data is compared with several other EOSs such as, Rohit Gupta EOS, Mie–Gruneisen EOS, Tait EOS, Murnaghan EOS, Birch–Murnaghan EOS,Vinet EOSandKholiya-Chandra EOS. Kholiya and Chandra[17] recently performed computational study on high-pressure compression behaviour of nanomaterials and provided good agreement with experimental data at high pressure also verified by average deviations.

Table 1 Shows values of B_0, B'_0, and B''_0 and average percentage deviations from Eq. (1).

S. No.	Nanomaterial	B_0 (GPa)	B'_0	B''_0	Max Pressure (GPa)	Reference
1	TiO_2 (anatase)	190.4	4	0.470	16.72	[18]
2	Ni (20 nm)	185	4	0.122	33.40	[19]
3	CdSe (rock salt phase)	74	4	0.360	8.00	[20]
4	AlN (Hexagonal)	321	4	0.481	14.5	[21]
5	3C-SiC (30 nm)	245	2.9	0.128	23	[22]
6	Rb_3C_{60}	17.35	3.9	0.277	0.66	[23]

Results and Discussions

Second order bulk modulus (B''_0)are calculated for TiO_2 (anatase), Ni (20 nm), CdSe (rock salt phase), AlN (Hexagonal), 3C-SiC (30 nm) and Rb_3C_{60} nanomaterials and finding pressure for various points with respect to volume for several nanomaterialequation of states like, Rohit Gupta EOS, Mie–Gruneisen EOS, Tait EOS, Murnaghan EOS, Birch–Murnaghan EOS Vinet EOS and Kholiya-Chandra EOS. The data for all nanomaterials defined from three constants such as B_0, B_0' and B_0'' are listed in table 1. The second order bulk modulus B_0'' are calculated from equation (1). Under compressions of such nanomaterials (TiO_2 (anatase), Ni (20 nm), CdSe (rock salt phase), AlN (Hexagonal), 3C-SiC (30 nm) and Rb_3C_{60}) pressures and its validity test arecalculated againfrom Eq. (1) and several other isothermal EOSs Eq. (2 to 7). Microsoft Office software has been used to do the calculations.

The results obtainedfrom these EOSs are presented in Fig. 1 to 6 in terms between pressure and(V/V_0) and its experimental data from.[18-23] Eq. (1) gives better agreement such as compared with the other EOSs. The obtained results compared with experimental data show in Figs. 1 to 6, thesevalues calculated from using Eq. (1) and closer to experimental data of nanomaterials. The experimental uncertainty result provided by Sharma and Kumar[2] with experimental measured P–V data is often pressuring calibration errors, therefore, we considered Eq. (1) calculation for the compression behavior of TiO_2 (anatase), Ni (20 nm), CdSe (rock salt phase), AlN (Hexagonal), 3C-SiC (30 nm) and Rb_3C_{60}. The results are reported in Fig. 1 to 6 along with the experimental data[18-23] and these corresponding results are presented in Table 1. Significantly, the results are showing better agreement with the experimental data.

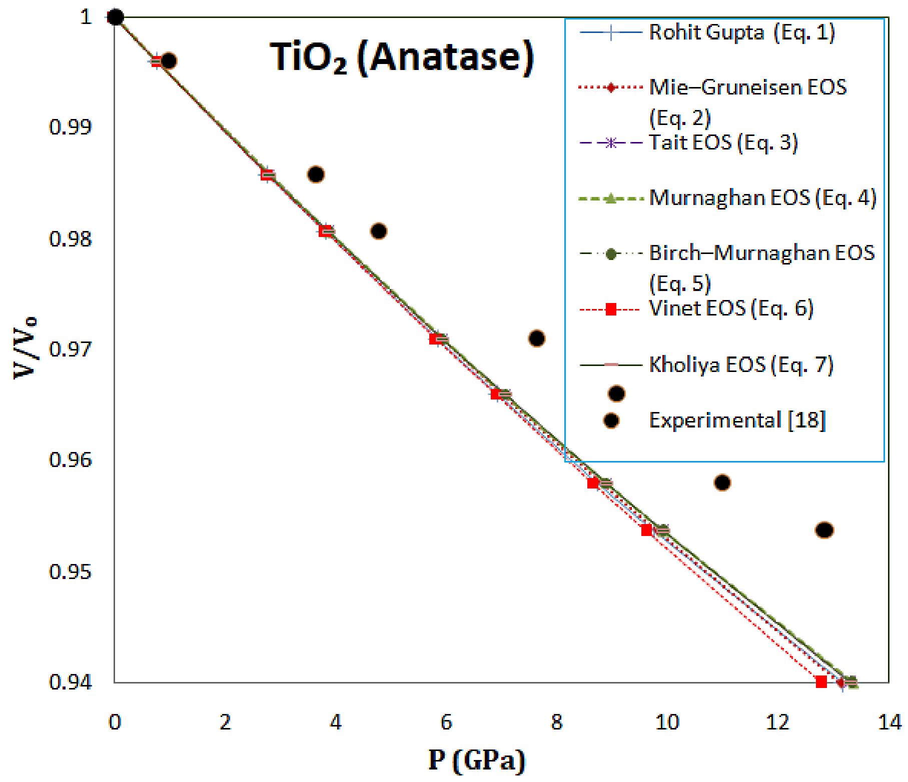

Fig. 1: Several EOSs are used for calculating high-pressure behaviour V/V_0 for TiO_2 (Anatase).

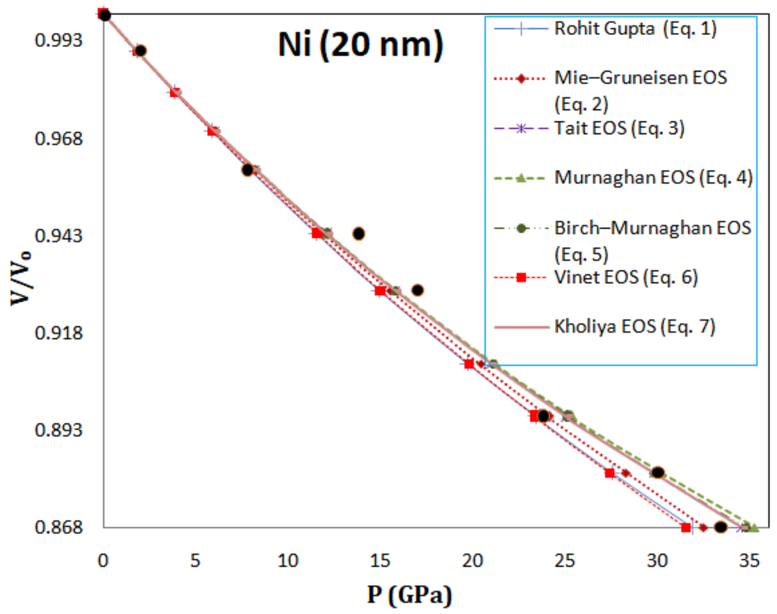

Fig. 2: Several EOSs are used for calculating high-pressure behaviour V/V₀ for Ni (20 nm).

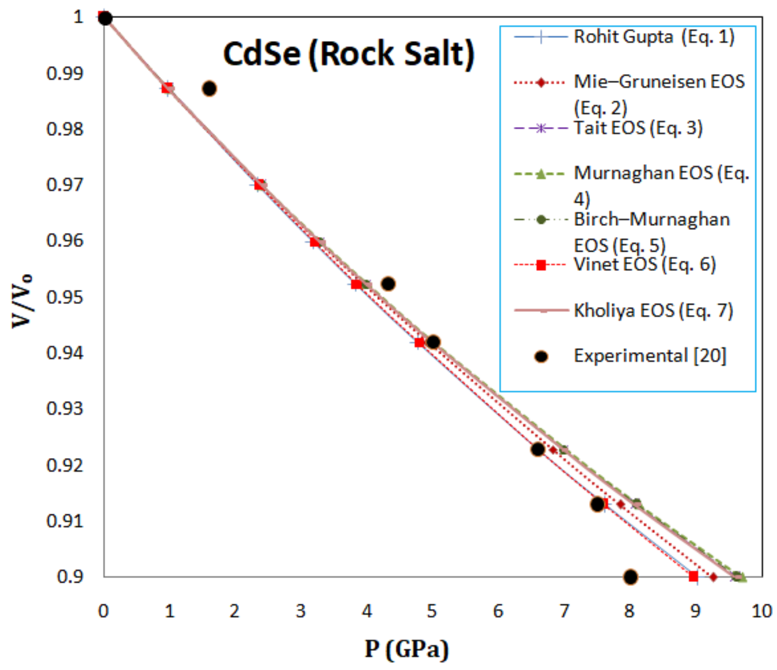

Fig. 3: Several EOSs are used for calculating high-pressure behaviour V/V₀ for CDSE (Rock Salt).

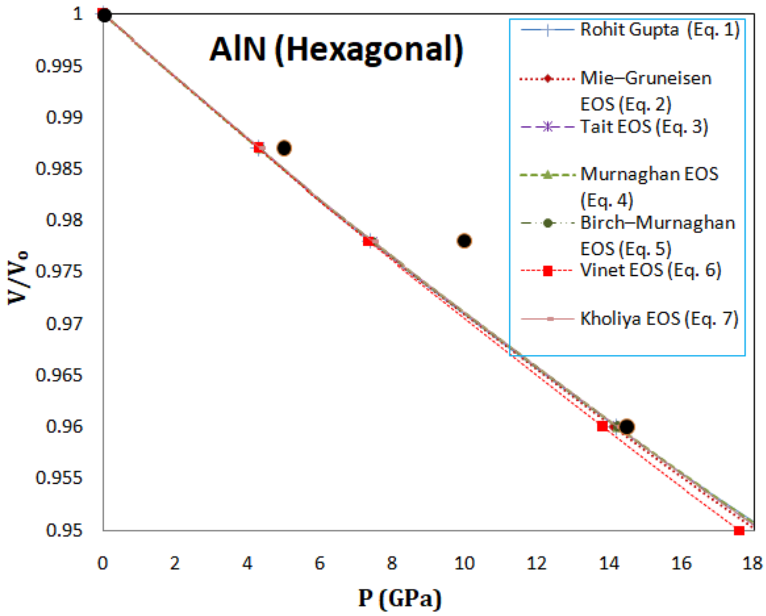

Fig. 4: Several EOSs are used for calculating high-pressure behaviour V/V_0 for AlN (Hexagonal).

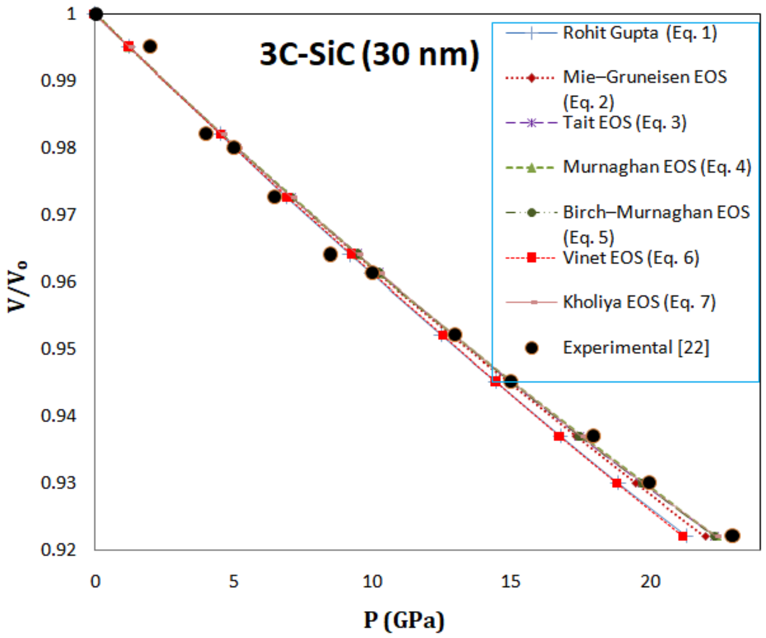

Fig. 5: Several EOSs are used for calculating high-pressure behaviour V/V_0 for 3C-SiC (30 nm).

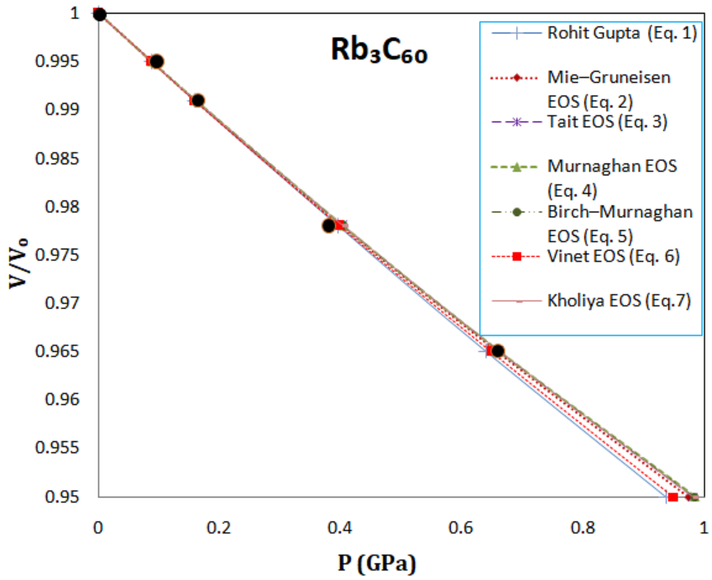

Fig. 6: Several EOSs are used for calculating high-pressure behaviour V/V₀ for Rb_3C_{60}.

Conclusion

Second order pressure derivative of bulk modulus EOS for nanomaterialsare predicted by our previous EOS study. EOSs for nanomaterials aremuch useful under high pressure compression behavior of nanomaterials and solids. The major advantages of these EOSs are that the experimental data is not available. Therefore the given studies for nanomaterials must be helpful under high-pressure compression behavior because at this level arrangement of experimental setup don't easy task. The results give better deal compare with experimental data and EOSs data, it is clear from figure 1 to 6. Present work is simple and effective method to study compression behaviour of nanomaterials and solids.

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Conflicts of Interest

The authors declare no competing interests.

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