# Study of high pressure compression in nanomaterials

**Monika Goyal & B.R.K.Gupta**

***Abstract*— In the present study ,the high pressure compression behavior of some of the nanomaterials such as 3C-SiC (30 nm), TiO2 (rutile phase),Ge (13 nm), γ- $Si_3N_4$, MgO (100nm),Ni (20 nm), $C_{60}$ Solid has been studied using two parameter based isothermal equations of state ,i.e. ,Birch Murnaghan EOS(BMEOS), Murnaghan EOS (MEOS),usual Tait's equation of state ,Vinet EOS, Kholiya EOS, Sharma and Kumar EOS .The results obtained 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 the present approach.**

***Index Terms*— Nanomaterials; Equations Of State; Compression; Isothermal Bulk Modulus; First Pressure Derivative of Bulk Modulus.**

## I. INTRODUCTION

The nanomaterials are very sensitive to external parameters like pressure and temperature. The study of nanoparticles 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. Over the past few years a large number of new materials with large hardness values have been fabricated [1, 2].Nanomaterials exhibit many promising characteristics on the aspect of their mechanical, thermal and electronic properties as compared to their respective bulk materials. The structural phase transtion and elastic behavior of nanomaterials under pressure have been of great interest and widely investigated in the high pressure research field. It is observed that under high pressure, the nanomaterials show very interesting properties because of following reasons: (i) modification of interactions between nano-object and pressure transmitting medium, (ii) transformation of nano-constitutive elements, and (iii) transformation of the interactions between nano-object due to drastic change in surface-volume ratio of atoms. This is why the pressure induced studies on nanomaterials have attracted the attention of the researchers working in this field.

During past few years, several experimental studies have been carried out to study the high pressure effect on nanomaterials.Nanocrystalline Nickel (20nm) was studied experimentally under high pressure by Chen et al.[3] using X-ray diffraction method. Study of nanocrystalline rutile type ( $TiO_2$ ) has been carried out using X-ray diffraction technique at ambient temperature upto 47.4 GPa by Olsen etal. [4].Liu etal. [5] synthesized nanocrystalline 3C-SiC (30 nm) by laser –induced vapour phase reactions and performed the energy dispersive X-ray diffraction experiment at room temperature using Si oil as a pressure transmitting medium to obtain quasi hydrostatic condition. Kiefer etal. [6] investigated the volume compression and elastic properties of γ phase of $Si_3N_4$ crystal under the effect of high pressure. Rekhi etal [7] studied the compressibility in MgO with particle size 100 nm. In the present study the authors have calculated the volume compression in nanomaterials 3C-SiC (30 nm), $TiO_2$ (rutile phase), Ge (13 nm), γ- $Si_3N_4$, MgO (100nm), Ni (20 nm),$C_{60}$ Solid, using equations of state such as Birch Murnaghan EOS (BMEOS), Murnaghan EOS (MEOS), usual Tait's equation of state , Vinet EOS, Kholiya EOS, Sharma and Kumar EOS . The method of analysis is given in section 2.The results are discussed in section 3.

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## II. .METHOD OF ANALYSIS

The usual Tait's equation of state gives non linear relation of compression and pressure for different class of solids and liquids. The Tait's equation of state is obtained by assuming the fact that the product of thermal expansion coefficient ($\alpha_T$) and bulk modulus ($B_T$) is constant under the effect of pressure [10], i.e.

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

Differentiation of equation (1) with respect to volume at constant temperature gives

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

Anderson –Gruneisen parameter is defined as

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

where $\delta_T$ is Anderson –Gruneisen parameter at constant temperature T.

From equation (2) and (3), we get

$$\delta_T = \frac{V}{\alpha}\left(\frac{d\alpha}{dV}\right)_T = -\frac{V}{B}\left(\frac{dB}{dV}\right)_T \qquad (4)$$

Assuming $\delta_T$ to be independent of V,

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

Anderson-Gruneisen parameter $\delta_T$ and η = V/$V_o$ (where $V_o$ is the initial volume) are related by the following relation [11],

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

Where A is a constant for a given nanomaterial. In view of equation (6), equation (4) can be written as

$$\frac{dB}{B} = \left[\frac{-A}{V_o} + \frac{1}{V}\right] dV \qquad (7)$$

Integrating eq. (7), we get

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

Where B is equal to

$$B = -V\left(\frac{dP}{dV}\right)_T \qquad (9)$$

sing equation (8), equation (9) can be represented as

$$\frac{B}{B_o} \exp A\left[1 - \frac{V}{V_o}\right] dV = -dP \qquad (10)$$

The integration of equation (10) gives

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

Here $B_o$ is the bulk modulus at zero pressure and the constant A is determined from the initial conditions, i.e. at V= $V_o$,

$$A = \delta_T^o + 1$$

On substitution of constant A in equation (11) and taking natural log, we get the following final form of usual Tait's equation of state,

$$V(P,T_o)/V(o,T_o) = 1 - \frac{1}{B_o^{'}+1}\log\left[1+\left\{\frac{B_o^{'}+1}{B_o}\right\}P\right]$$

(12)

Where $V(P,T_o)$ 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 $T_o$. $B_o$ and $B_o^{'}$ are the isothermal bulk modulus and its first pressure derivative at T = $T_o$.

The most widely used EOS for the study of high pressure compression in nanomaterials is the third order Birch Murnaghan EOS(BMEOS),which reads as follows[12]:

$$P = \frac{3B_o}{2}\left[\left(\frac{V_o}{V}\right)^{\frac{7}{3}} - \left(\frac{V_o}{V}\right)^{\frac{5}{3}}\right]\left[1+\frac{3}{4}(B_o^{'}-4)\left\{\left(\frac{V_o}{V}\right)^{\frac{2}{3}}-1\right\}\right]$$

(13)

Murnaghan noted in his general theory of finite strain[10] that bulk modulus varies linearly with pressure. Murnaghan EOS(MEOS) reads as follows:

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

Vinet EOS used to study some properties of nanomaterials reads as follows[13]:

$$P = 3(1-\chi)B_o[\exp\eta(1-\chi)\ ]/\chi^2 \qquad (15)$$

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

Sharma and Kumar formulism is developed by considering pressure P as a function of relative change in volume [14] reads as follows:

$$P = B_o\left(1-\frac{V}{V_o}\right) + B_o\left(\frac{B_o^{'}+1}{2}\right)\left(1-\frac{V}{V_o}\right)^2 \qquad (16)$$

To study high pressure compression in nanomaterials, Kholiya framed an EOS [15] which reads as follows:

$$P = \frac{B_o}{2}\left[(B_o^{'}-3) - 2(B_o^{'}-2)\left(\frac{V}{V_o}\right)^{-1} + (B_o^{'}-1)\left(\frac{V}{V_o}\right)^{-2}\right]$$

(17)

Equations (12-17) are used to study the compression behavior in nanomaterials.

## 3. Results and Discussion

In the present investigation the author have determined the volume compression in nanomaterials under the effect of high pressure by making use of different isothermal equations of state (12-17).the equation of state employed in the present study consists of only two input parameters, viz. $B_o$ and $B_o^{'}$ .we have compiled these data in table 1 along with their proper references. Equations (12-17) are used to study the compression behavior in nanomaterials and the calculated results are shown in figure 1-6 along with the experimental data for the sake of comparison. It is found that the usual Tait EOS gives better agreement with the experimental values for all nanomaterials especially at lower pressure range. On the basis of overall description, it may be emphasized here that the present approach is capable of explaining the compressional and elastic properties of nanomaterials under high pressure satisfactorily. Due to simplicity and applicability, this may be of the current interest to the researchers engaged in the study of elastic properties of nanomaterials under high pressure.

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Table 1:
Value of input parameters used in the present work.

| Nanomaterials | $B_o$(GPa) | $B_o^{'}$ | Ref. |
|---|---|---|---|
| Ni (20 nm) | *185* | 4 | [3] |
| 3C-SiC (30 nm) | 245 | 2.9 | [5] |
| $TiO_2$ (rutile phase) | 211 | 8 | [4] |
| Ge (13 nm) | 92 | 4 | [8] |
| γ- $Si_3N_4$ | 339 | 4 | [6] |
| MgO (100nm) | 179 | 1.5 | [7] |
| | | | |
| $C_{60}$ Solid | 18.1 | 5.7 | [9] |

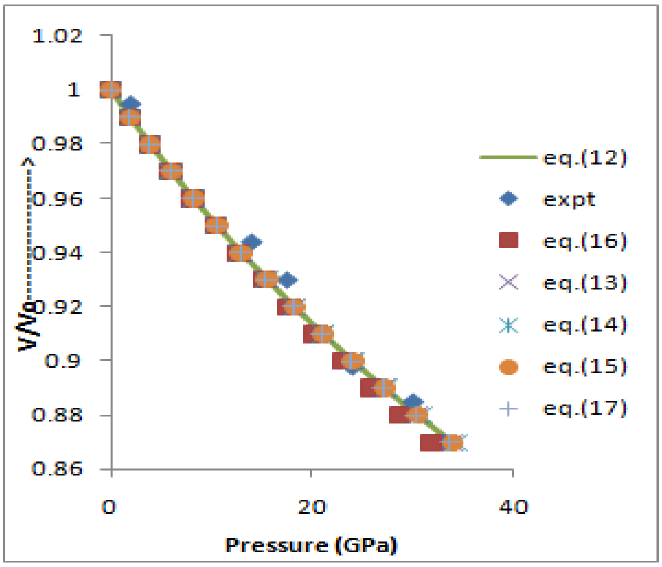


Figure1:Pressure dependence of $\frac{V}{V_o}$ for nanocrystalline nickel(20nm)

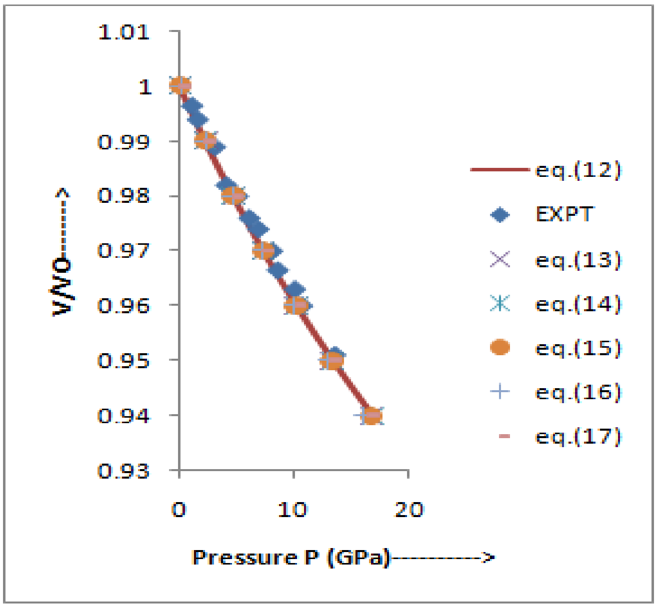


Figure2:Pressure dependence of $\frac{V}{V_o}$ for $TiO_2$ (rutile phase)

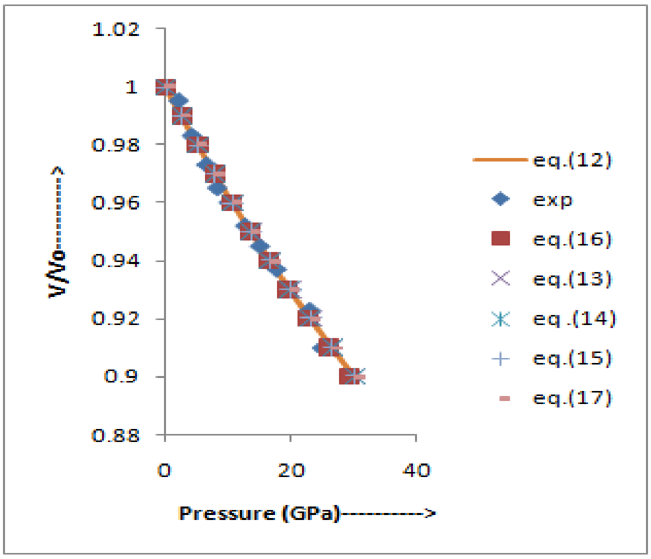


Figure 3:Pressure dependence of $\frac{V}{V_o}$ for 3C-SiC (30 nm)

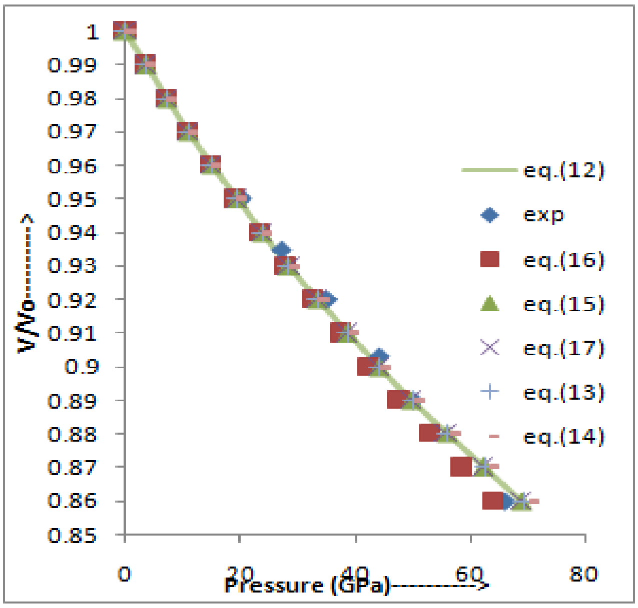


Figure 4:Pressure dependence of $\frac{V}{V_o}$ for γ- $Si_3N_4$

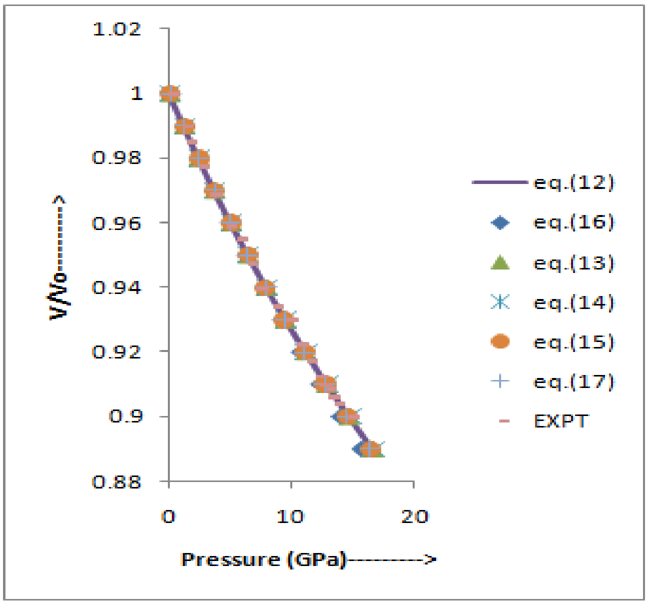


Figure5: Pressure dependence of $\frac{V}{V_o}$ for Ge (13 nm)

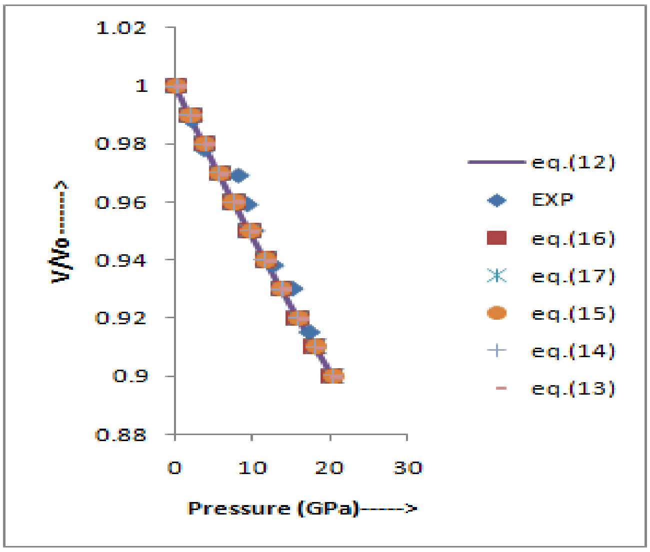


Figure 6: Pressure dependence of $\frac{V}{V_o}$ for MgO

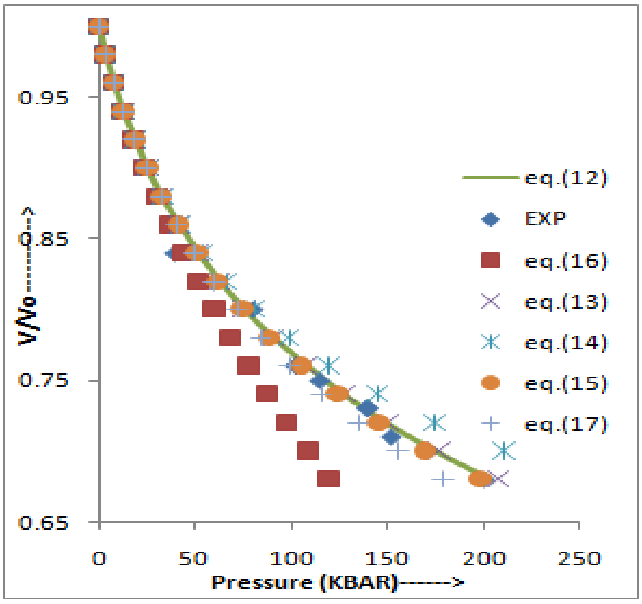


Figure7: Pressure dependence of $\frac{V}{V_o}$ for $C_{60}$ solid