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Study of Nanomaterials Under Second Order Bulk Modulus

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***Abstract:** In this study, we analyze the variation of pressure under different values of $\left(\frac{V}{V_0}\right)$ for nanomaterials using second order pressure derivative of bulk modulus equation of state. Second order pressure derivative of bulk modulus show fine studies of nanomaterials. The Gupta & Gupta EOS is used to calculate the resultant data of ε-Fe (Hexagonal iron), α-Fe_2O_3 and Ni-filled MWCNT nanomaterials and compared with other equations of state, like Tait EOS, Mie–Gruneisen EOS, Vinet EOS and experimental data available in literature. The resultant data show good agreement with experimental data and other EOSs.*

***Keywords:** Nanomaterials; Bulk Modulus; Nanocrystalline; Volume Expansion; High Pressure.*

I. INTRODUCTION

Nanomaterials are expected to be the turning point of the next technological revolution in solid-state electronics, to emerge as new structural materials, the nonomaterial described in principle as material of which a single unit small sized between 1 to 100 nm. Material science-based approach to nanotechnology to serve as systems for controlled drug delivery and to have a considerable impact in practically all domains of science. The nanomaterials are very sensitive to external parameters like pressure, volume, and temperature. The pressure temperature and volume research has developed an interdisciplinary area that has important applications in various fields of science one of the important outputs of the experiment is pressure volume temperature relationship terms EOS can determine various properties of nanomaterials under varying conditions of pressure volume and temperature [1-3]. The formulation of bulk modulus of the second-order pressure derivative with thermal expansivity is derived by Rohit Gupta et al. [4]. Nanomaterials have attracted the attention of researchers because of their wide applications [5, 6], their properties and structure stability display many differences as compared with bulk materials because of its small size.

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Recently researchers have much attention to nanomaterials because the temperatures of nanomaterials are different from that of the corresponding bulk materials. The melting temperature of nanomaterials with free surface decreases with a decrease in the crystal size [7-12]. There is evidence that the nanomaterials and equation of state depend on the size [13, 14]. J. Diederichs et al. [16] suggest neutron diffraction studies of the compressibility of Rb_3C_{60} material by equation of state for DAC results show limited accuracy in pressure. B. Chen et al. [17] show the size effect on the bulk modulus possible for high-pressure phases, different-size nanocrystalline nickel under high pressure. J. Tang et al. [18] studied *X*-ray diffraction data with a synchrotron source by non-hydrostatic and quasi-hydrostatic conditions. Bulk modulus was found different during no phase transition was observed for either non-hydrostatic or quasi-hydrostatic compression for the pressure range of these experiments. High-pressure compression behavior of carbon nano-tubes has been studied experimentally.

Piermarini et al. [19] studied the hydrostatic properties of Fe_2O_3 nanocrystal revealing different behaviors under pressure was synthesized by micro emulation method in several systems of water, sodium, chloride, isopropyl pentane, pentane coated with one benzene sulphonic. The system suggests the qualitative nature in the characterization of quasi hydrostatic state. Z. jing et al. [20] Fe_2O_3 sample was characterized by using high-resolution transmission electron microscopy the nanocrystals are spherical there is a phase transition of Fe_2O_3 to Fe_2O_3 when the pressure reaches high. B. Chen [21][34][35][36] studied *X*- ray diffraction measurements on the nanocrystalline iron has been the subject of many experimental and theoretical parameter data for nanocrystalline Fe analysis of lattice grain growth was observed to occur under pressure.

Rekhi et al. [22] investigate the effect of particle size on the compressibility of MgO, Wang et al. [23] performed *X*-ray diffraction study on MgO at particle. H. Mao et al. [24] studied the EOS of nanocrystalline CuO using high energy synchrotron radiation and Raman spectroscopic techniques. Nanocrystalline Al_2O_3 was compressed quasi-hydro-statically to pressure up to 60GPa in a Mao-Bell type DAC, at room temperature, B. Chen et al. [25] the X-ray diffraction study has studied particle size effect on the compressibility of nanocrystalline aluminum room temperature at X-ray diffraction for nanocrystalline particle size result found that compressibility increases with decreasing particle size.

II. METHOD OF ANALYSIS

In this study the second-order bulk modulus equation of state (EOS) is used to determine the effect of pressure on nanomaterials, where P is a function of relative change in volume $\left(\frac{V}{V_0}\right)$ as follows [26]:

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

Tait EOS is studied for comparison purposes and will be described as follows [27]:

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

Mie–Gruneisen EOS reads as [28],

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

Vinet EOS reads as [29],

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

The experimental data are taken from Sharma and Kumar [30]. The experimental data show satisfactorily explains Eq. (12) for the high-pressure elastic behavior of nanomaterials. It is clear from the table and figures the calculated data less deviates from the experimental data. So the proposed equation is verified to analyze other nanomaterials.

Table-1: Shows Values of B0, B'0, and B''0 and Average Percentage Deviations using from Eq. (12)

Sl. No.	Nanomaterial	B_0 (GPa)	B'_0	B''_0	Max Pressure (GPa)	Average % Deviations (0 to Max Pressure)	References
1	ε-Fe (Hexagonal iron)	179	3.6	0.24	41.41	3.13	[31]
2	α-Fe_2O_3	336	4	0.192	32.20	3.53	[32]
3	Ni-filled MWCNT	190.4	4.0	0.36	18.40	2.92	[33]

III. RESULTS AND DISCUSSIONS

Second-order pressure derivative of bulk modulus EOS for nanomaterials are predicted by our previous studies. In this study, we predicted the second order pressure derivative EOS under different values of $\left(\frac{V}{V_0}\right)$ for ε-Fe (Hexagonal iron), α-Fe_2O_3 and Ni-filled MWCNT nanomaterials respectively, and compared with several other equations of state, like Tait EOS, Mie–Gruneisen EOS, Vinet EOS and experimental data available in the literature. The Gupta & Gupta EOS shows good agreement with experimental data. It is clear from table 1 and fig. 1, 2 and 3. The average percentage deviation is calculated under 0 to maximum pressure for ε-Fe (Hexagonal iron), α-Fe_2O_3 and Ni-filled MWCNT nanomaterials respectively 3.13, 3.53, and 2.92 using the maximum pressure 41.41, 32.20, and 18.40. So the EOS for second order pressure derivative of bulk modulus is used to find the fine studies of nanomaterials.

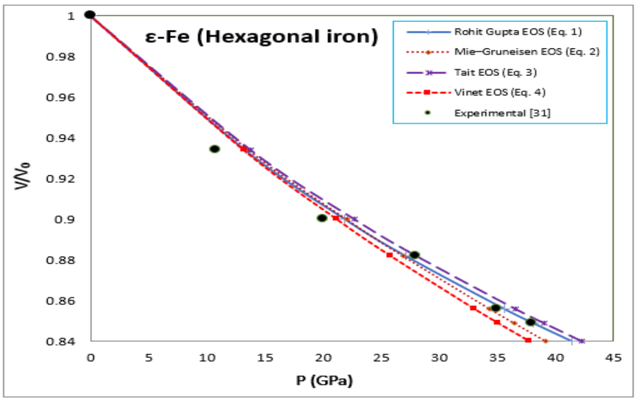

Fig. 1: Show High-Pressure Compassion Behavior of $\frac{V}{V_0}$ for ε-Fe (Hexagonal iron) Nanomaterial Using Study Under Several EOSs

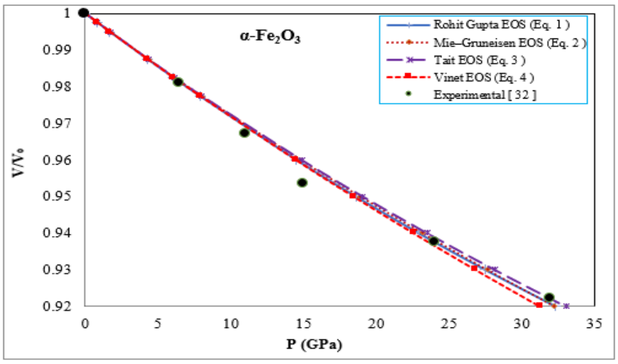

Fig. 2: Show High-Pressure Compassion Behavior of $\frac{V}{V_0}$ for α-Fe2O3 nanomaterial Using Study Under Several EOSs

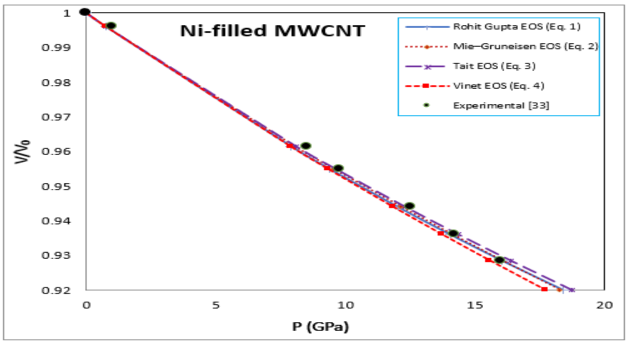

Fig. 3: Show High-Pressure Compassion Behavior of $\frac{V}{V_0}$ for Ni-filled MWCNT Nanomaterial Using Study Under Several EOSs

IV. CONCLUSIONS

The second-order pressure derivative of bulk modulus EOS is predicted by Gupta & Gupta. It is used to find the fine data for previous EOS of nanomaterials. So this EOS is very useful under the high-pressure compression behavior of nanomaterials. The major advantage of theoretical EOSs are that the experimental data is not available; we can calculate data from given EOSs. Therefore the EOSs are very useful under high-pressure compression behavior because at very high pressure the observation of experimental data is not easy. It is clear from that figures; that EOSs are a simple and effective method to find data under compression behavior of nanomaterials and solids.

DECLARATION STATEMENT

After aggregating input from all authors, I must verify the accuracy of the following information as the article's author.

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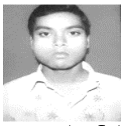

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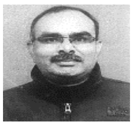

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