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Analysis of Volume Dependent Gruneisen Parameter of Nanomaterials using Equations of State

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Abstract— ***In our current study, we have made theoretical predictions for high pressure compression and the Grüneisen parameter under various compression conditions for nanomaterials. To achieve this, we employed two different equations of state (EOSs): the Murnaghan EOS and the Shanker EOS. The calculated values for pressure from both EOS align with established facts and serve as validation for our research. We obtain a new computing formula for the volume of the Grüneisen parameter γ at high temperatures. Applying this formula to nanomaterials such as*** $\gamma - Fe_2O_2$***, TiO2 (Rutile Phase), MgO (100 nm), 3C-SiC (30 nm), and Ge (Cubic) in different pressure ranges, we find that the calculated values of the Grüneisen parameter γ are in good agreement with the experimental value. Moreover, this agreement also suggests that these EOSs, commonly used for pressure calculations in bulk materials, can be effectively applied to nanomaterials as well. Additionally, we observed that the graph plotting the Grüneisen parameter against the volume compression ratio forms a similar curve for all nanomaterials. This finding is consistent with the existing knowledge that the ratio γ/Ω (where Ω=V/V0), representing the Grüneisen parameter to volume compression ratio, remains constant for nanomaterials. This further confirms the validity of our work.***

Keywords: EOS, Nanomaterial, Grüneisen Parameter, Volume derivative.

I. INTRODUCTION

The argument over the names associated with nanoscience and nanotechnology is dwindling in volume over time. On the other hand, it is increasingly common to refer to natural or artificial particles with at least one dimension of 100 nm or less as nanomaterials (NMs) and to particles with at least two dimensions between 1 and 100 nm as nanoparticles (NPs) [1].

Because of its special qualities, iron oxide is a desirable nanoparticle for use in biological applications. Specifically, γ-Fe2O3 nanoparticles can improve the therapeutic agent's permeability and stability across tissues, resulting in a prolonged circulation period. More specifically, various iron oxide formations Because of their high surface-to-volume ratio, nanocomposites are being used more often in the field of biomedical engineering [4].

Anatase, rutile, and brookite are the three crystal forms of TiO2. The functional characteristics, specific surface area, quantity of defects, phase transition temperatures, and stability of the various phases are all influenced by the size and shape of the TiO2 particles. In addition, the crystalline phase, crystallite size, and porosity of TiO2 affect its optical, textural, and catalytic properties. Consequently, because of the anticipated novel features, the synthesis of nanoparticulate TiO2 with customized specific surface area and high porosity for certain applications is of interest. According to research on TiO2 as a catalyst, anatase is the most effective phase in photocatalysis while rutile is the most effective phase in Sono catalysis [5 -6].

The elasticity of magnesium oxide (MgO), a typical oxide mineral and a potential lower mantle constituent, has been thoroughly investigated by researchers using a variety of techniques, including high-pressure ultrasonic studies, shock-wave compressions, and static compression in diamond anvil cells. The pressure dependence of the elastic constant has only been revealed by ultrasonic tests. It is clear that extrapolating the elasticity of MgO to lower mantle settings results in significant ambiguity when an uncertainty of 10% is present. Consequently, more precise measurements are needed to determine how MgO's elasticity depends on volume [7].

Due to its outstanding features, such as its huge bandgap, strong thermos conductivity, and high breakdown electric field strength, silicon carbide (SiC) has garnered significant attention as a viable semiconductor operating in complex environments. Additionally, it is thought to be a viable option for high-precision devices including quantum computing applications, optical instruments, and micro-electromechanical systems (MEMS). However, it is technically challenging due to SiC's great hardness and brittleness. Understanding the deformation behaviour and anisotropy effect of 3C-SiC is made possible by this research [8].

No previous studies have investigated the variation of the Grüneisen parameter with increasing compression. Since the Grüneisen parameter's value at various compressions is essential for the use of nanomaterials in contemporary technology, that is the main focus of our attention [9].

II. METHODS AND ANALYSIS

Anderson pointed out [10] that the Anderson–Grüneisen parameter $\delta(T,P)$, the second Grüneisen parameter q and the first pressure derivation of the bulk modulus $B_T^{/}$ satisfy the following relation at high temperature:

$$\delta(T,P) = q + B_T^{/} - 1 \tag{1}$$

For many solids linear relation between bulk modulus and pressure provides

$$B_T^{/} = B_0^{/}$$

$$\text{So } \delta(T,P) = q + B_0^{/} - 1 \tag{2}$$

Researcher proposed a linear relationship for the volume dependence of the Anderson–Grüneisen parameter [11].

$$\delta(T,P) + 1 = A\,\eta \tag{3}$$

where A is a constant at given reference temperature, i.e., A = $\delta_{T0} + 1$

Where δ_{T0} is the Anderson–Grüneisen parameter at P = 0 and on reference temperature. According to Eqs. (2) and (3), at high temperature we get

$$q = A\,\eta - B_0^{/} \tag{4}$$

Second Grüneisen parameter q is defined as

$$q = \left(\frac{\partial \ln \gamma}{\partial \ln V}\right)_T$$

$$\left(\frac{\partial \ln \gamma}{\partial \ln V}\right)_T = A\,\eta - B_0^{/}$$

On integrating

$$\gamma = \gamma_0 \left(\frac{\exp[A(\eta-1)]}{\eta^{B_0^{/}}}\right) \tag{5}$$

The compression ratio η in Eq. (5) can be calculated from the different equation of states (EOS).

Birch Murnaghan EOS [12]

$$\eta = \left[1 + \frac{B_0^{/}}{B_0} P\right]^{-\frac{1}{B_0^{/}}} \tag{6}$$

Or

$$P = -\frac{B_0}{B_0^{/}}\left[1 - (\eta)^{-B_0^{/}}\right] \tag{7}$$

ShankerEOS [13].

$$\eta = 1 + \frac{1 - \left(1 + 2P\left(\frac{B_0^{/}+1}{B_0}\right)\right)^{\frac{1}{2}}}{B_0^{/}+1} \tag{8}$$

Or

$$P = B_0\left[\left(1 - \frac{V}{V_0}\right) + \left(\frac{B_0^{/}+1}{2}\right)\left(1 - \frac{V}{V_0}\right)^2\right] \tag{9}$$

III. RESULT AND DISCUSSION

Table 1. Input Parameters utilized in this research [11-17]

S.N.	Nanomaterials	B_0	$B_0^{/}$	A	Gruneisen Parameter (γ_0)[14]
1	$\gamma - Fe_2O_3$	374[15]	4[15]	5	1.67
2	$T_iO_2(Rutile\ Phase)$	211[16]	8[16]	9	3.67
3	MgO(100nm)	179[17]	1.5[17]	2.5	0.42
4	$3C - SiC(30nm)$	245[18]	2.9[18]	3.9	0.62
5	$G_e(Cubic)$	74.9[19]	3[19]	4	0.67
6	$\propto -F_e(Nanotubes)$	89.7[20]	20.9[20]	21.9	9.62

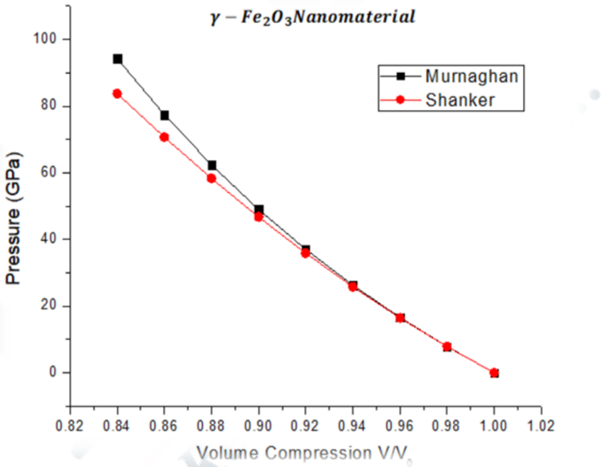

Fig 1. Variation of Pressure with Compression of $\Upsilon - Fe_2O_3$ Nanomaterial by Murnaghan and Shanker EOS

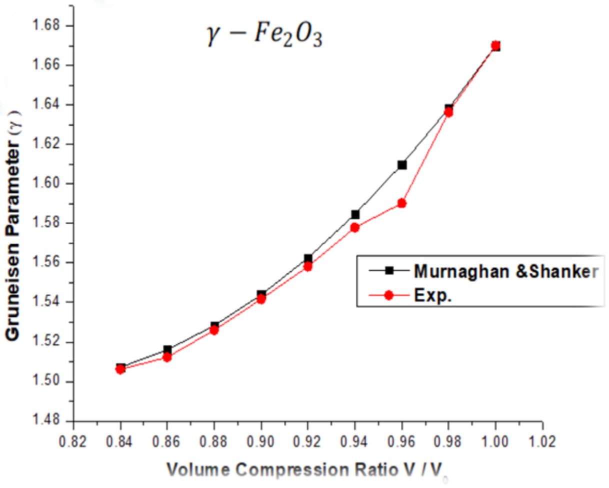

Fig 2. Variation of Gruneisen Parameter (ϒ) of $\Upsilon - Fe_2O_3$ Nanomaterial with Compression by Murnaghan and Shanker EOS with Exp. [21]

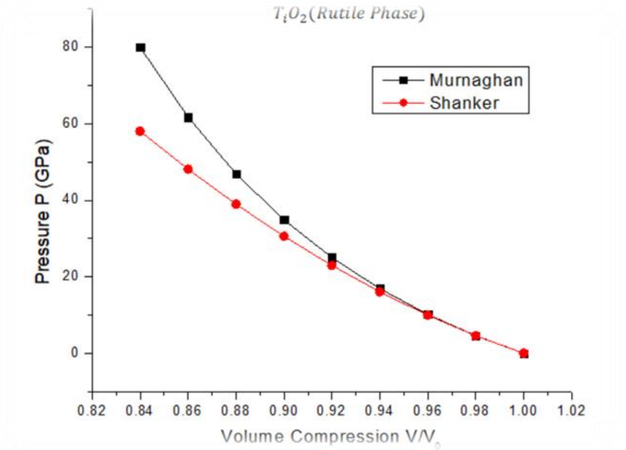

Fig 3. Variation of Pressure with Compression of TiO_2 (Rutile phase) Nanomaterial by Murnaghan and Shanker EOS

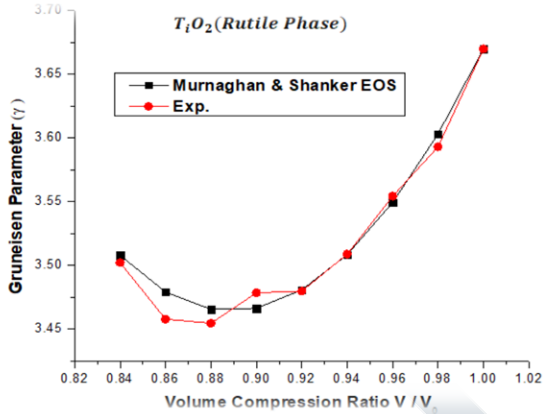

Fig 4. Variation of Gruneisen Parameter (ϒ) of T_iO_2 (*Rutile phase*) Nanomaterial with Compression by Murnaghan and Shanker EOS with Exp. [22]

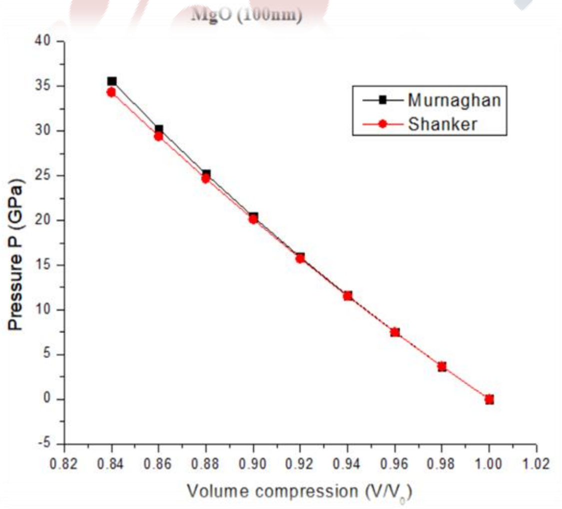

Fig 5. Variation of Pressure with Compression of MgO (100nm)Nanomaterial by Murnaghan and Shanker EOS

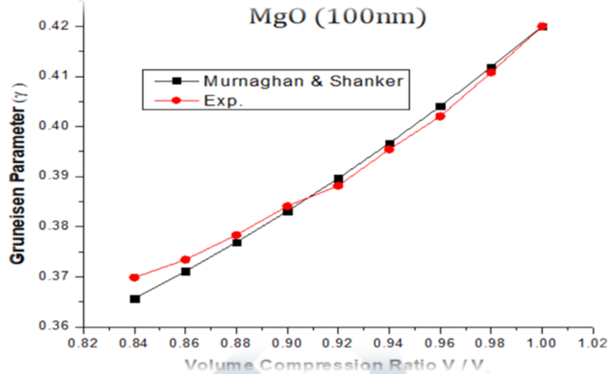

Fig 6. Variation of Gruneisen Parameter (ϒ) of MgO (100nm)Nanomaterial by Murnaghan and Shanker EOS with Exp. [23]

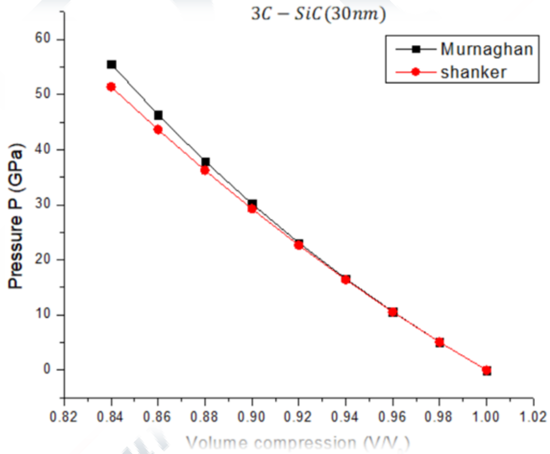

Fig 7. Variation of Pressure with Compression of 3C-SiC (30nm) Nanomaterial by Murnaghan and Shanker EOS

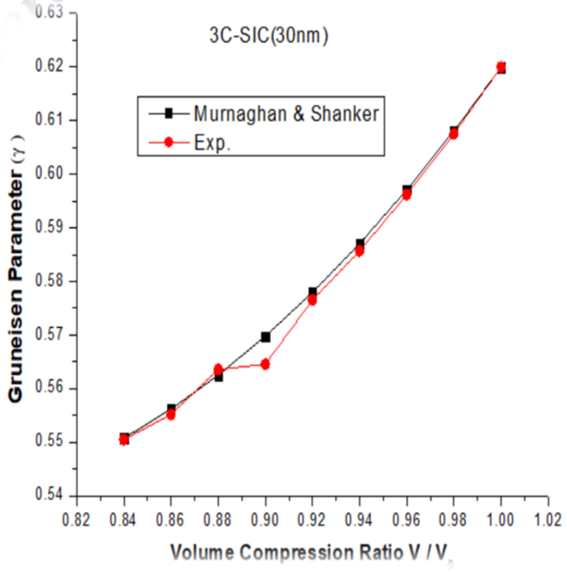

Fig 8. Variation of Gruneisen Parameter (ϒ) of 3C − SiC (30nm)Nanomaterial with Compression by Murnaghan and Shanker EOS with Exp. [24]

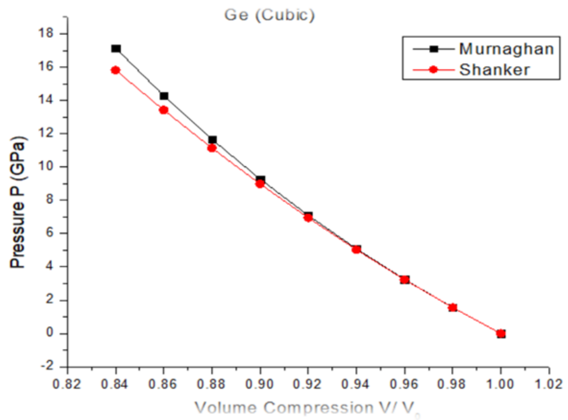

Fig 9. Variation of Pressure with Compression of Ge (Cubic) Nanomaterial by Murnaghan and Shanker EOS

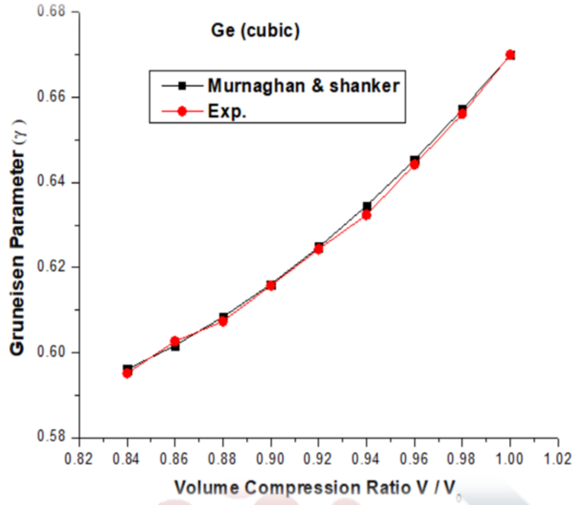

Fig 10. Variation of Gruneisen Parameter (ϒ) of Ge (Cubic) Nanomaterial with Compression by Murnaghan and Shanker EOS with Exp. [25]

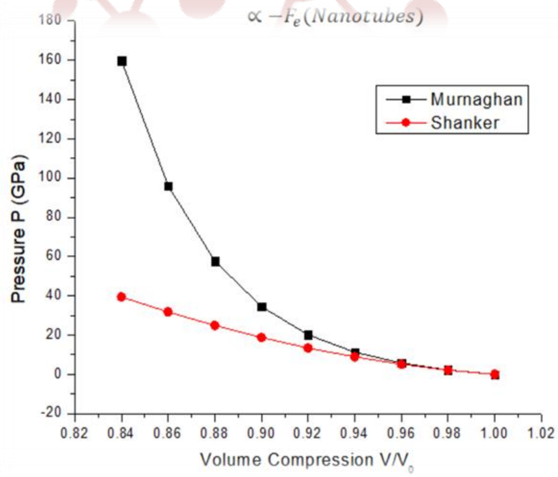

Fig 11. Variation of Pressure with Compression of $\alpha-Fe(Nanotubes)$ Nanomaterial by Murnaghan and Shanker EOS

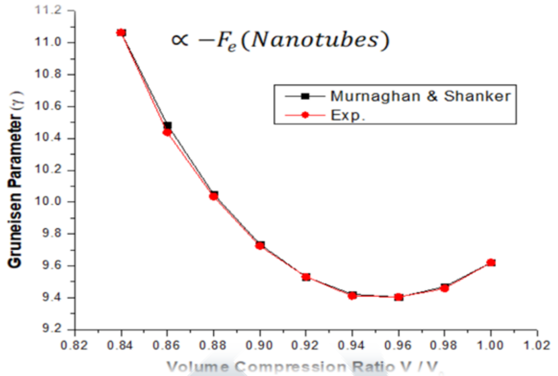

Fig 12. Variation of Gruneisen Parameter (ϒ) of $\alpha-Fe$ (Nanotubes) with Compression by Murnaghan and Shanker EOS with Exp. [26].

In the present work we have described two different forms of EOS; equations (7) and (9). Equation (7) corresponds to Murnaghan EOS, equation (8) corresponds to Shanker EOS. All the two EOS contains only two parameters B_0 and B_0' both at zero pressure. These values of B_0 and B_0' have been recommended by [12]-[17]. The value of A can be obtained by fitting the experimental data on the Grüneisen parameter at high temperature and high pressure. Using the parameters mentioned above, we calculate the values of the Grüneisen parameter of taken nanomaterials in this research .The values of pressure P for nanomaterials, TiO_2(Rutile Phase), MgO (100nm), 3C-SiC(30nm), Ge(Cubic), were computed for given increments of V/V0 by using equation (7) and (9). The value of input parameter, B_0 and B_0', are taken from literature displayed in table-1. Using the value of volume compression ratio V/V_0 and zero compression Gruneisen parameter taken from literature$_0$ and B_0' both at zero pressure. These values of B_0 and B_0' have been recommended by [11], the volume dependence Gruneisen parameter computed from equations (5) for nanomaterials, and dependency variation are displayed in Fig 1. – Fig 12.

In all Figures It is found that the calculated pressure of the nanoparticle decreases with decrease of compression and Gruneisen parameter goes to increases. At low compression value, all curves with the two EOSs are relatively close to each other. The result of compression by both EOSs significantly close up to relative compression of .94 for all nanoparticle. Increasing compression values beyond .94 causes the curves of all nanomaterials by both EOSs exhibit divergence .The divergence is more marked in pressure with relative volume of TiO_2 (Rutile phase) and greatly differ with Murnaghan EOS and shanker EOS comparison to other nanomaterials . The trend of variation of Gruneisen parameter with relative volume with Murnaghan EOS & shanker EOS are similar to all compression and reaches to minimum value at compression =.84 of nanomaterials , MgO (100nm), 3C-SiC (30nm),Ge(Cubic),but for nanomaterials TiO_2 (Rutile Phase), at compression =.84 & at =.96. Volume dependence of Gruneisen parameter of nanomaterials, MgO

(100nm), 3C-SiC (30nm), Ge (Cubic), decreases with increase of compression but of nanomaterials increases with increase of compression to a value 11.0, but for TiO_2 (Rutile Phase) variation is remarkable first decreases up to compression =.88 & increases to 3.50 at maximum compression taken in this research. Results and discussion. In this paper, we obtain new relations for the volume dependence of the Grüneisen parameter γ.

IV. CONCLUSIONS

In this paper, we obtain new relations for the volume dependence of the Grüneisen parameter γ. By comparing our theoretical results calculated from Murunaghan & shanker EOS, we can see that the calculated results of, TiO_2 (Rutile Phase), MgO (100nm), 3C-SiC (30nm), Ge (Cubic), are in good agreement with them (see Fig 2-7). By comparing our theoretical results with experimental data for five nanomaterials, we can see that the calculated results are in good agreement with the experimental results (see in Fig.2-7).

Since the new study provides results that are fairly close to the experimental data for nanomaterials, it may be especially helpful for analysing the volume dependence Gruneisen parameter solids, particularly nanomaterials. Therefore, the present formulation could be helpful in developing volume dependence Gruneisen parameter experiments on the compression behavior of nanomaterials in the future.

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