Theoretical high pressure study for bulk and nano carbon using different EOSs

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Abstract

Volume compression behavior of graphite and SWCNT have been investigated under high pressure using Birch-Muranghan, Vinet, Sigh-Kao and Kholiya-Chandraequation of state(EOSs).The obtained results have been compared with available experimental data . Combing these different EOSs with Grünesein approximation theoretical evaluation of phonon density of state, for both graphite and SWCNT, under the effect of high pressure, obtained results show the importance of considering the variation of Grünesein parameter under high pressure .

Keywords NanoCarbon, SWCNT, High pressure, Phonon frequency spectrum, EOSs

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1 Introduction

Single-Wall carbon nano tube (SWCNT) and low dimensions systems are promising systems both for pure science and applications. Most of their physical properties depend on corresponding lattice dynamics using inelastic neutron scattering over a large phonon energy range 0-225 meVAlvarez .L(Alvarez et al.2000) present the first vibrational density of state.Hone(Hone et al.2000) presents theoretical phonon density of states for SWCNT and graphite. EOSs have been used in studying C_{60}(Singh and Kao2013).In the present work a theoretical high pressure study performed for studying the behavior of nanomaterials. Using EOSs at high pressure, allow interpolation and extrapolation to the regions for which experimental data are not available.

Well known EOSs expressed by Birch-Murnghan and Vinet further to EOSs developed by (Kholiya et al. 2014 ; Wang et al.2000) have been used to evaluate compressed volume V/V0 for SWCNT and graphite. Combined this EOSs with Grünesein approximation have been used in ,present work, to determine the behavior of phonon frequency spectrum of SWCNT and graphite under high pressure. The Grünesein parameter has both macroscopic and miroscopic definitions (Birch1952) in terms of thermodynamic as given in equation 1 as:

$$\gamma = \frac{\alpha_v B_o}{C_v \rho} \quad \text{---(1)}$$

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.

Where

α_υ is the volume coefficient of thermal expansion.

is the density.

B_0 - isothermal bulk modulus at ambient conditions .

C_{υ}- specific heat at constant volume

ρ- density

The microscopic definition arises from vibration of atoms in a solid, as the vibrational frequencies of the individual atom in a solid varied with volume V via the relationshown in eqution 2 .

$$\gamma = -\frac{\partial \ln \omega}{\partial V} \text{---(2)}$$

where

ω is the frequency of vibration.

This introduce for a relation for pressure (volume) dependence of Grünesein parameter which will be used in present work for the improvment of calculated density of state functions under high pressure

2 Theoretical Details

Equations of state

Four EOSs have been used in present work to investigate graphite and SWCNT. These are the well known Birch-Murnaghan EOS, Vinet EOS, further to high pressure EOSs for nanomaterials which are expressed in their formal form as follow:

(i) Birch-Murnaghan EOS(Birch1952).

$$P_{BM} = \frac{3B_0}{2}\left[(\frac{V}{V_0})^{-\frac{7}{3}} - (\frac{V}{V_0})^{-\frac{5}{3}} \right]\left[1 + \frac{3}{4}(B_0^{'} - 4)\left((\frac{V}{V_0})^{-\frac{2}{3}} - 1 \right) \right] \text{------------(3)}$$

.

Where

P_{BM} - the lower subscript refer to Birch-Murnaghan EOS,

P is the pressure.

B_0 - isothermal bulk modulus at ambient conditions.

B_0' - first derivativ e of B_0 for pressure.

V - volume under high pressure P.

V_0 – volume initial (atmospheric) pressure.

(ii) Vinet EOS (Vinet et al.1987)

$$P_V = 3B_0(\frac{V}{V_0})^{-\frac{2}{3}}\left(1 - (\frac{V}{V_0})^{\frac{1}{3}} \right)\exp\left[\left\{ \frac{3}{2}(B_0^{'} - 1) \right\}\left\{ 1 - (\frac{V}{V_0})^{\frac{1}{3}} \right\} \right]. \text{---------(4)}$$ \Where

P_υ - the lower subscript refer to Vinet EOS, P is the pressure.

(iii) Singh and Kao (Singhand.Kao2013)

$$P_{S-K} = B_0(1-\frac{V}{V_0}) + \left\{\frac{B_0(B_0^{'}+1)}{2}\right\}(1-\frac{V}{V})^2 \quad (5)$$

Where

$P_{S\text{-}K}$-the lower subscript refer to sigh and KaolEOS ,P pressure

(iv)Kholiya and Chandra EOS (Chandra andKholiya 2016).

$$P_{K-C} = B_0\left[(1-\frac{V}{V_0}) + \frac{5}{2}(1-\frac{V}{V_0})^2\right] \quad \text{--------------------(6)}$$

Where
$P_{K\text{-}C}$the lower subscript refer to Kholiya and Chandra EOS , P pressure

Grünese in Approximation

When high pressure impressed on solids, lattice vibrations modified in a very complex way in which it is difficult to calculate these changes.However, the Grunesein approximation simplifies the matter by looking to the context that in principle specific volume of solids will be compressed under the influence of high pressure, this volume compression inducing strain within the crystal and the symmetry of the lattice may be change and consequently there will be a shiftting in the equilibrium position of lattice vibrations. Using Grünesein approximation (Dlouha 1964) give expressions for the changes in lattice vibrations frequencies and in mode density due compression in volume as:

$$\nu_P = \nu_0\left(\frac{V}{V_0}\right)^{-\gamma} \quad \text{---------------------------------- (7)}$$

Where

ν_P frequency at pressure P.

ν_0 frequency at pressure P=0

γ Grünesein approximation

$$g_P(\nu, V_P) = \left(\frac{V}{V_0}\right)^{\gamma} g\left[\nu\left(\frac{V}{V_0}\right)^{\gamma}, V\right]$$

----------------(8)

Where

Mode density at pressure P $g(\nu, V_P)$

3 Calculation and Results

Evaluation of compressed volumes

On using graphite and SWCNT values tabulated in Table 1 within the different EOSs given in equations (3-6).

Table 1 Values of B_0, B'_0, γ for graphite and SWCNT(Goncharov 1991)

Material	Bulk Modulus		Ref	Grünesein parameter	Ref
	B_0 GPa	B'_0		γ	
Graphite	33.8	8.9	(Hanfland etal 1989)	1.33	(Goncharov 1991)
SWCNT	133.00	5.3	(Singh 2012)	1.33	

obtained results for variation of V/V_o under high pressur for both graphite and SWCNT aretabulated in Table 2and3 and shown in Figs. 1 and 2 respectively.

Table 2 Compressed volume V/V_o for graphite evaulated by uasing different EOSs in comparison with exprimentai data

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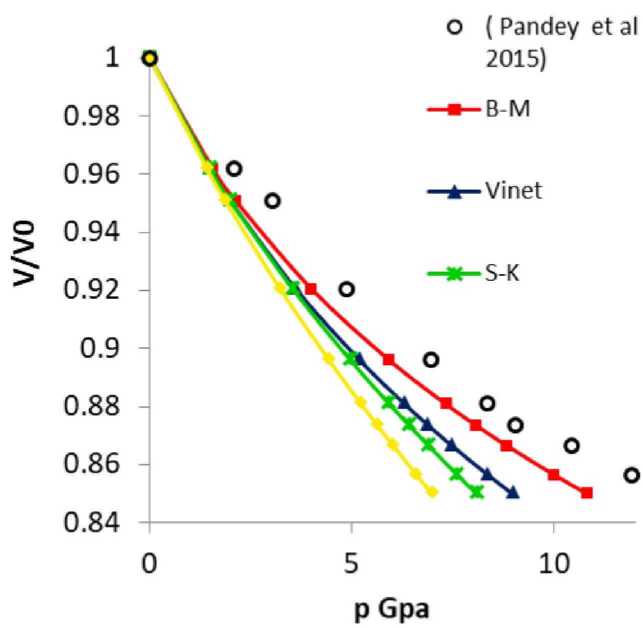
V/V_o	PressureExp. Data PGpa(Pandey*et al .,)*	Pressure calculated using different EOSs P Gpa			
		B-M	vinet	S-K	k-c
1	0	0	0	0	0
0.9618	2.087	1.560801	1.484745	1.485983	1.414466
0.9507	3.0434	2.12899	1.996894	1.990835	1.871716
0.9205	4.8696	3.994594	3.608188	3.530917	3.221161
0.8961	6.9565	5.906738	5.178363	4.953088	4.424015
0.8809	8.3478	7.316632	6.297361	5.919394	5.224196
0.8737	9.0434	8.050597	6.86917	6.39865	5.616858
0.8665	10.434	8.830483	7.469615	6.891749	6.01828
0.8566	11.913	9.982774	8.344556	7.592361	6.584541
0.85	13.913	10.80573	8.961288	8.073975	6.97125

Table 3 Compressed volume V/V_0under higp pressure for SWCNT evaualted by uasing different EOSs in comparison with exprimental data .

V/V_0	Pressure Exp. Data P Gpa(Pandey et al 2015)	Pressure calculated using different EOSs P Gpa			
		B-M	Vinet	S-K	K-C
1	0.328	0	0	0	0
0.996102	1.016393	0.905297	0.900456	0.905192	0.905192
0.991142	2.032787	2.083329	2.058408	2.082521	2.082521
0.987008	3.016393	3.087637	3.033674	3.085246	3.085246
0.98311	4.032787	4.053818	3.961887	4.048673	4.048673
0.979094	5.016393	5.069252	4.927126	5.059566	5.059566
0.977087	6.032787	5.584705	5.413161	5.571967	5.571967
0.972126	7.016393	6.880723	6.623804	6.857776	6.857776

Fig.1 and Fig.2 show variation ofV/V_0 under high pressure for both graphite and SWCNT respectively.



and Debye temperature and phonon frequency shift (

Fig 1 Compressed volume V/V_o for graphite using different EOSs in comparison with experimental data(Pandey et al 2015) .

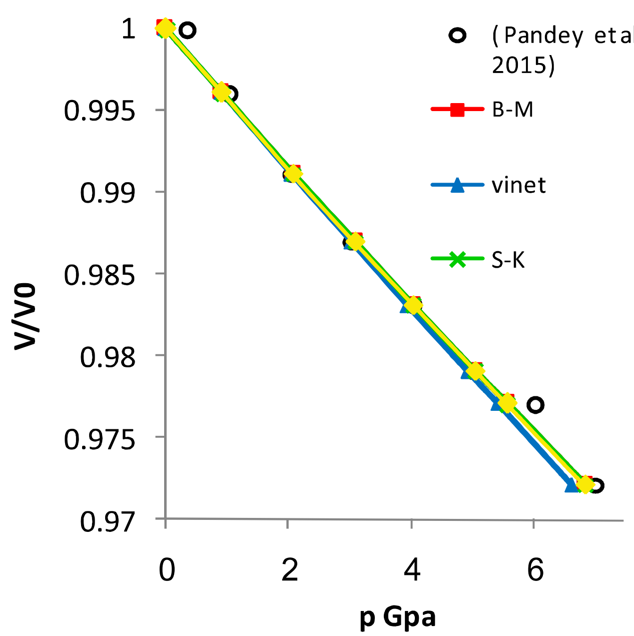
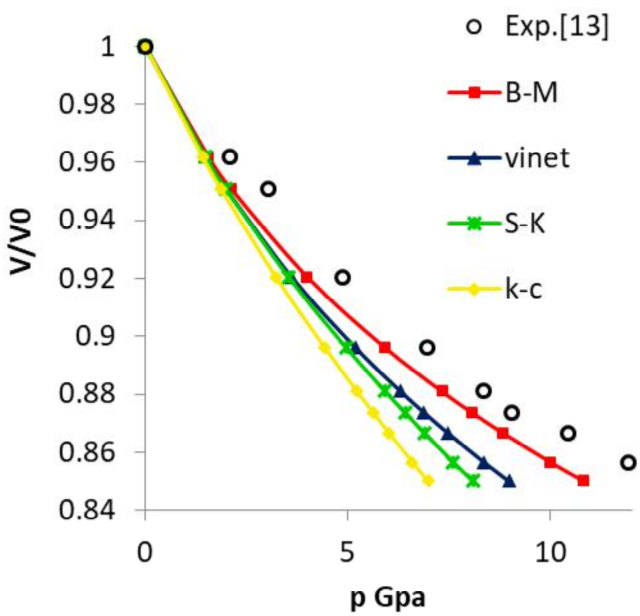


Fig 2 Compressed volume V/V_o for SWCNT using different EOSs in comparison with experimental data(Pandey *et al.*, 2015) .



Calculations of phonon density of states under high pressure

Theoretical phonon density of states for graphite and SWCNTshow in Fig.3(Hone et al 2000).

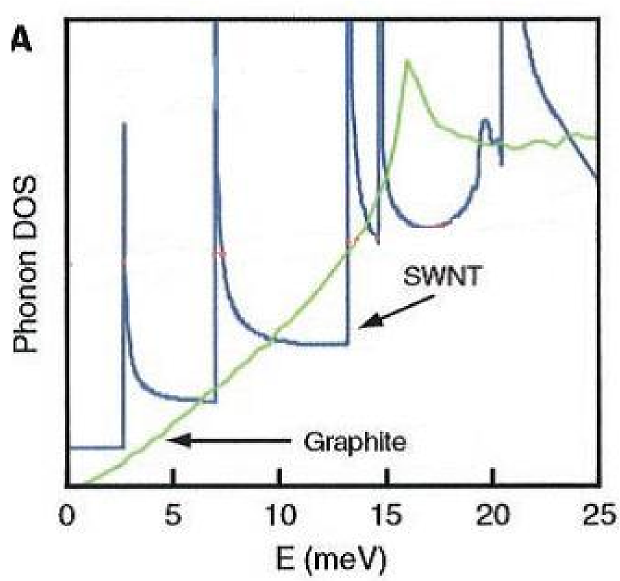


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Fig.3 Phonon distribution functions for graphaite and SWCNT(Hone et al 2000).

Both of the phonon distribution functions have been calibrated, using Matlab ,where the corresponding $g(\nu)$ for each ν have been recorded . Using equations 7 and 8 with for different V/V_o values (different pressure) and γ values of graphite and SWCNT from Table 1.Figs 4 and 5 show variation of phonon distribution functions for graphite and SWCNT under high pressure ,respectively, according to different EOSs.

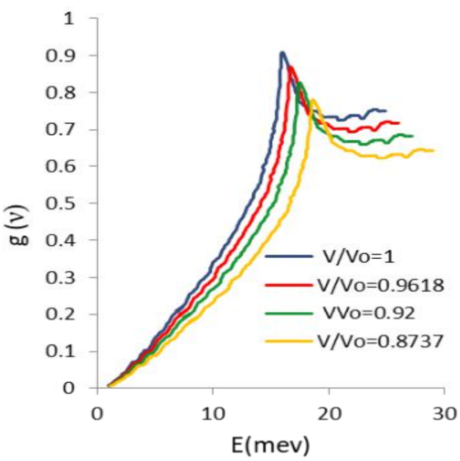

Fig. 4 Variation of graphite PDOS under high pressure according to different EOSs.

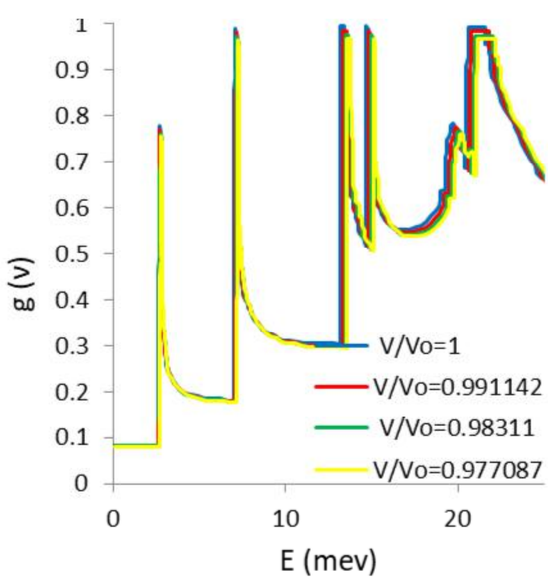

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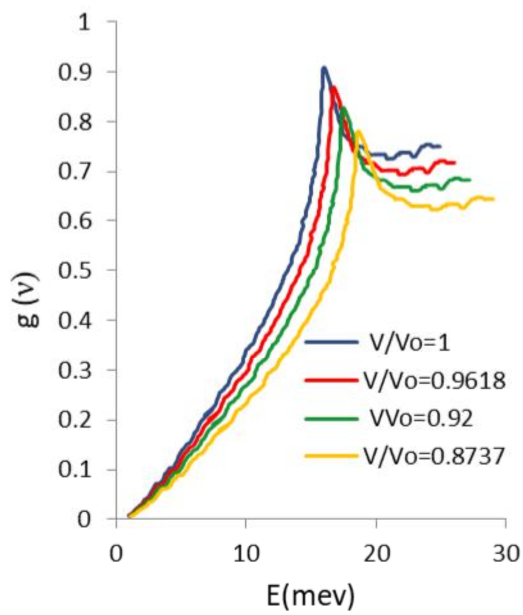
Fig. 5 Variation of SWCNT PDOS under high pressure according to different EOSs.



Calculations of γ pressure dependence

As consequence of Eq 2 pressure depends of γ parameter had been formulated as :(Boehler and Ramakrishnan 1980)

$$\gamma_p = \gamma\left(\frac{V}{V_o}\right)^q \text{------------------} (9)$$

Where

γ_p- Grünesein parameter at pressure p.

q- Second Grünesein parameter. Considered to equal one in present work.

Following (.Al-sheikh andAl-saqa 2019) an improvement for variation phonon density of state achieved on considering pressure dependence of γ- parameter from Eq 9 . Figs.6 and 7 show variation of γ- parameter with pressure for graphite and SWCNT respectively .Combining eq.(9) with both equations 7 and 8. Figs. 8 and 9 show modified results for variation of density of state functions, for graphite and SWCNT, under high pressure respectively.

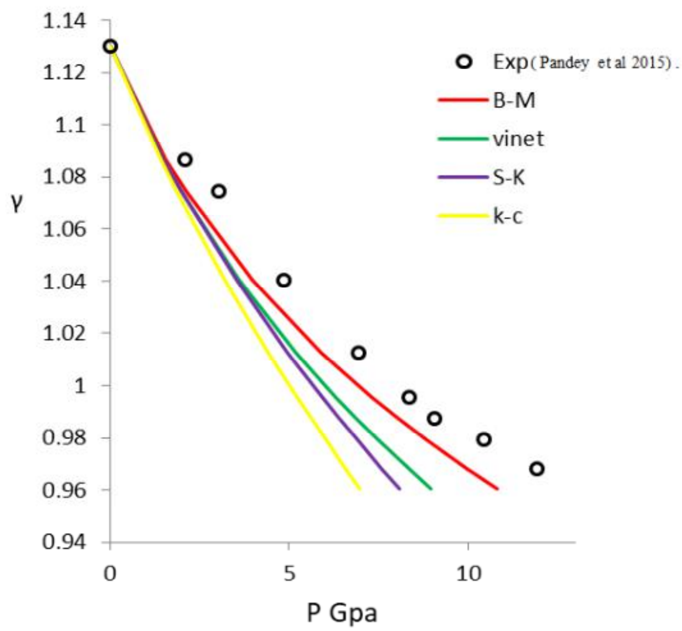


Fig.6 Variation of γ- parameter under high pressure for graphite .

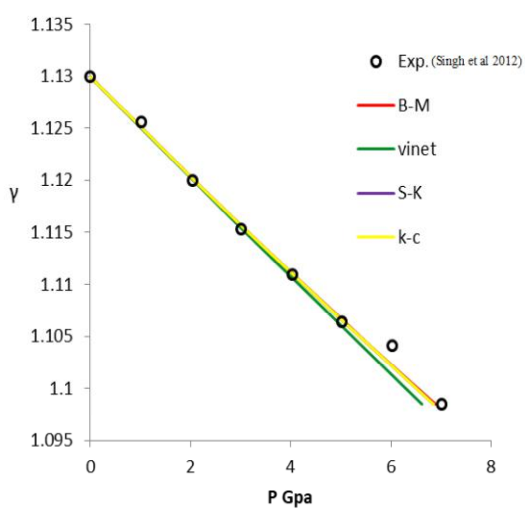


Fig. 7 Variation of γ- parameter under high pressure for SWCNT. .

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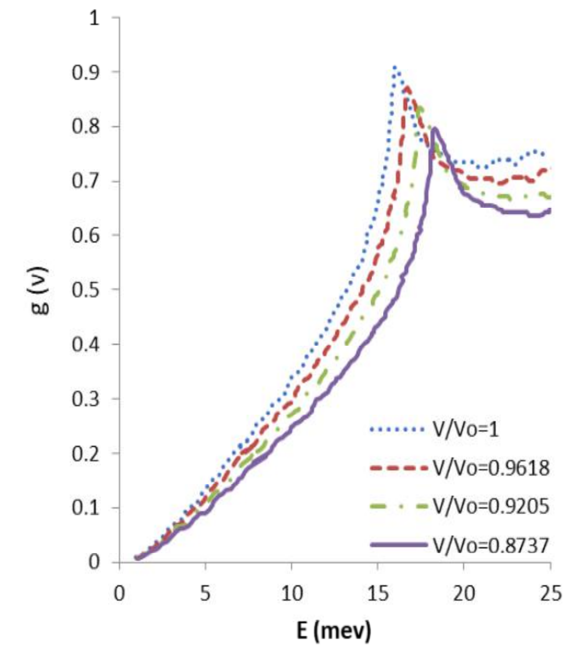

Fig. 8 Improved variation of graphite PDOS under high pressure according to different EOSs considering ɣ pressure dependence .

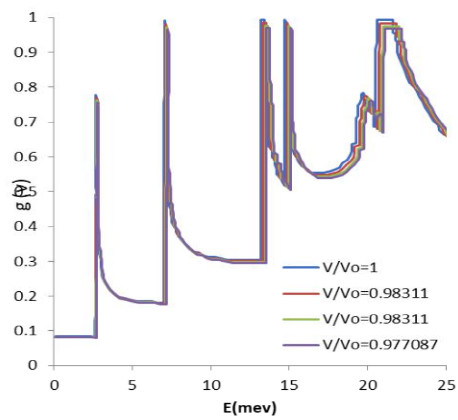

Fig. 9 Improved variation of SWCNT PDOS under high pressure according to different EOSs considering γ pressure dependence

4 Discussion

1-Figs1and2.show that the results of V/Vo variation under the influence of high pressure in both graphite and SWCNT calculated by using B-M EOS were the closest to the experimental data compared to the results obtained from the rest of EOSs applied in present work including S-K and K-C, although they are two EOSs for nanomaterials.

2- Figures 4 and5 show that the effect of pressure on PDOS for both graphite and SWCNT has led to an expansion of the distribution function towards higher energies and this expansion increases with increase of high pressure applied.

3-The consideration of γ pressure dependence when performing calculations of PDOS variation under high pressure as shown in Figures 8 and 9 was reflected in the reduction of the expansion of the phonon distribution functions toward higher energies.

5 Conclusions:

1-The results of present work showed the possibility of using the well known EOSs, such as B-M EOS, used for bulk materials to perform calculations of nanomaterials after taking into consideration the values of parameters of nanomaterial under investigation.

2- The expansion of PDOS towards higher energies under the influence of high pressure, means that vibrational frequencies in solids shifted towards higher frequencies. This is consistent with what (Sherwood,1972) mentioned that the applied high pressure on solid converts some inactive vibrational modes into active vibrational modes.

3-Reduction in the shifting of PDOS frequencies towards the higher frequencies after taking into account γ parameter pressure depence, is consistent with what Alsheik and Alsaqa, 2019 reached when studying gold under pressure.

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