

Variation of the Structural Properties of IV Element Nano Clusters Due to Tensile Stress

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ABSTRACT

CNDO/2 method with 27 unit cells composed of 216 atoms, has been used for calculating and studying the lattice constant, density, total energy, cohesive energy, bulk modulus, microhardness, Young modulus, speed of sound, acoustic phonons energy, plasmon energy and vibrational energy, for diamond, silicon, germanium, and gray tin subjected to tensile stress. And to investigate the categories of these clusters; do these clusters have properties of nano materials or properties of bulk materials? It is found that most values of the investigated properties decrease with tensile stress except the lattice constant and the vibrational energy. In addition, two simple formulas have been established for both the bulk modulus and plasmon energy. It is found that the investigated clusters show bulk behavior.

Keywords: IV Elements; Structural Properties; Pressure; Nano Materials

1. Introduction

The general properties of IV materials make them useful in many fields [1-3], such as the field of electronics [4-6]. So these materials have been extensively investigated [7-13]. The variation of material properties with pressure is an interesting field [14-15]. So, the first motive of the present work is to investigate the effect of pressure on some properties of diamond, silicon, germanium, and gray tin. The second motive is to answer the following question: Could the 216 atom clusters of these elements be regarded as nano materials or bulk materials concerning the structural properties?

A LUC (Large Unit Cell) composed of 27 unit cells (each of these units contains 8 atoms) has been used in the present analysis. The CNDO/2 method with STO (Slater Type Orbital) and LCAO (Linear Combination of Atomic Orbitals) approximation [16] was used to calculate the lattice constant, cohesive energy, total energy, and bulk modulus of the aforementioned elements. The Young modulus, microhardness, speed of sound, energy of phonons and plasmons have been also determined.

2. Calculations

The orbital exponent (ξ), bonding parameter (β), *s*-shell electronegativity (*EES*), and *p*-shell electronegativity (*EEP*), shown in **Table 1** for the four elements, are the pa-

Table 1. Parameters of CNDO/2 for C, Si, Ge and α -Sn.

		Diamond			
Par. (eV)	Pres.	Ref. [16]	Ref. [17]	Ref. [18]	Ref. [19]
ξ	1.76	1.652	1.83	1.765	1.820
$-\beta$	10.48	21	10	10.2	10.24
<i>-EES</i>	7.3	14.05	5.57	7	6.220
<i>-EEP</i>	5.55	5.572	4.39	5.5	4.352
		Silicon			
Par. (eV)	Pres.	Ref. [16]	Ref. [17]	Ref. [18]	Ref. [20]
ξ	1.56	2.075	1.635	1.54	1.59
$-\beta$	14.41	13.06	5.45	6.4	6.2
<i>-EES</i>	6.755	10.03	7.25	6.3	7.25
<i>-EEP</i>	4.479	4.133	4.95	4.5	5
		Germanium			
Par. (eV)	Pres.	Ref. [16]	Ref. [17]	Ref. [21]	
ξ	1.304	1.527	1.98	1.98	
$-\beta$	9.35		5.35	5.352	
<i>-EES</i>	9.35		9.35	9.357	
<i>-EEP</i>	5.4		5.4	5.404	
		Grey tin			
Par. (eV)	Pres.	Ref. [16]	Ref. [17]	Ref. [22]	
ξ	1.3	1.425	2.05	1.996	
$-\beta$	13.03		5.35	5.334	
<i>-EES</i>	9.35		9.46	9.452	
<i>-EEP</i>	4.4		4.69	5.632	

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rameters used in the CNDO/2 method [16] to calculate the lattice constant (a_o), cohesive energy (E_c) and total energy (E_o) in the ground state (zero pressure-temperature) [z-PT].

The calculated structural properties compared with other results are shown in **Table 2**. Our results were fitted according to Equation (1), the state equation of Murnaghan,

Table 2. The structural properties of C, Si, Ge, and α -Sn.

Element	a_o (Å)			B_o (GPa)		
	Pres.	Theo.	Exp.	Pres.	Theo.	Exp.
C	3.556	3.56 [19] 3.56 [17]	3.556 [23]	433.59	520 [19] 808 [17]	433 [23]
Si	5.4309	5.43 [17]	5.431 [23]	98.93	149.5 [17] 180.8 [20]	98 [23]
Ge	5.6579	5.65 [17] 5.65 [21]	5.658 [23]	86.096	137.8 [17] 103 [21]	75 [23]
Sn	6.4809	6.46 [17] 6.487 [22]	6.481 [23]	53.084	96.6 [17] 100 [22]	53 [23]
Element	E_{coh} (eV)			v_o m/s		
	Pres.	Theo.	Exp.	Pres.	Theo.	Exp.
C	7.3722	7.36 [19] 7.55 [17]	7.37 [24]	11089.155	15159 [17]	19161 [19]
Si	4.6319	4.68 [17]	4.63 [24]	6517.4732	8010 [17] 6600 [25]	9150 [25]
Ge	3.8501	3.85 [17] 3.83 [21]	3.85 [24]	4022.8669	5070 [17] 3830 [25]	5400 [25]
Sn	3.1447	3 [17] 3.14 [22]	3.14 [24]	3033.9389	4095 [17]	
Element	P_{max} (GPa)	$\rho_o \times 10^{-3}$ (Kg/m ³)	E_{ZPV} (eV)	E_{pl} (eV)		
				Pres.	Theo.	Obs.
C	1110 [26]	3.526 [27]	0.215 [24]	31.19739		
Si	11.7 ^h	2.329 [27]	0.065 [24]	16.60106	16.4 - 16.9 [27]	16 [27]
Ge	10.6 ^h	5.32 [27]	0.036 [24]	15.640944	16 - 16.4 [27]	16 [27]
Sn	1 ⁱ	5.767 [27]	0.021 [24]	12.713636		
Element	B'_o	θ (K)				
C	3.553 [23]		2220 [24]			
Si	4.153 [23]		674 [24]			
Ge	4.678 [23]		374 [24]			
Sn	4.804 [23]		220 [24]			

in order to estimate the change of energy $E(V)$ with pressure [30].

$$E(V) = E_o + \frac{B_o V}{B'_o} \left[\left(\frac{V_o}{V} \right)^{\frac{B'_o}{B_o}} + 1 \right] - \frac{B_o V_o}{B'_o - 1} \quad (1)$$

This change, using Equation (2), determines the change of vibrational energy (F_{vib}) [26] as below:

$$P_T = - \frac{\partial E(V)}{\partial V} - \frac{\partial F_{vib}}{\partial V} \quad (2)$$

where P_T is the isothermal pressure, V_o and B_o are the volume and bulk modulus of the unit cell at [z-PT], and V is the volume at any pressure.

The bulk modulus at [z-PT] is calculated using Cohen empirical formula [31]:

$$B_o = \frac{1970 - 200I}{d^{3.5}} \quad (3)$$

where I is the ionicity factor which equals 0, 1 and 2 for IV, III-V and II-V groups respectively [31], and d ($= 0.433 a$) is the intratomic distance [23], where a is the lattice constant at any pressure.

Then both the isothermal bulk modulus at any pressure (B_T), Equation (4) [32], and the derivative of bulk modulus at zero pressure (B'_o), Equation (5) [23,33], have been calculated as:

$$B_T = -V \frac{dP_T}{dV} \quad (4)$$

$$B'_o = \left. \frac{dB}{dP} \right|_{P=0} \quad (5)$$

By solving Equations (4) and (5), one can get:

$$V = V_o \exp(-\varphi) \quad (6)$$

where

$$\varphi \equiv \frac{P_T}{B_o + B'_o P_T} \quad (7)$$

The results of volume vs pressure are shown in **Figure 1**, in comparison with:

- Murnaghan equation of state EOS [34] of pressure (P_M);

$$P_M = \frac{B_o}{B'_o} \left[\left(\frac{V_o}{V} \right)^{\frac{B'_o}{B_o}} - 1 \right] \quad (8)$$

- Birch-Murnaghan EOS of pressure (P_{BM});

$$P_{BM} = \frac{3}{2} B_o \left[\left(\frac{V_o}{V} \right)^{\frac{2}{3}} - \left(\frac{V_o}{V} \right)^{\frac{5}{3}} \right] \left\{ 1 - \frac{3}{4} (4 - B'_o) \left[\left(\frac{V_o}{V} \right)^{\frac{2}{3}} - 1 \right] \right\} \quad (9)$$

- Vinet EOS of pressure (PBM) [35];

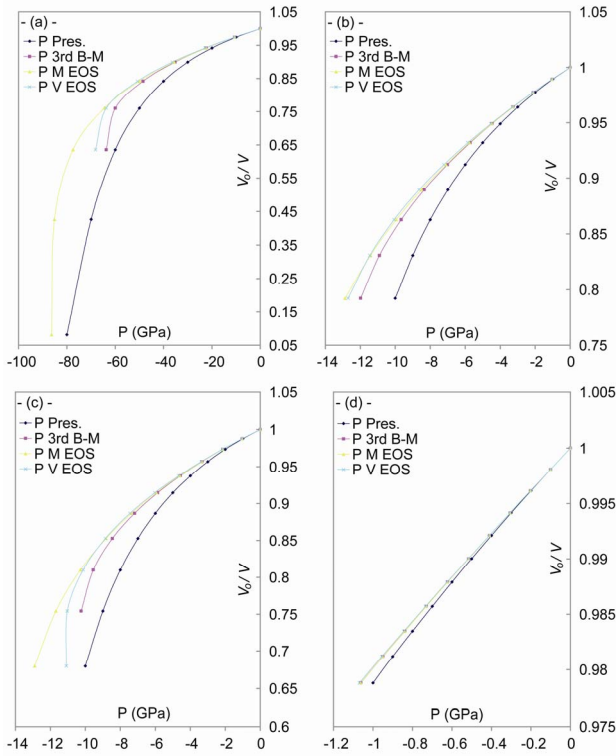


Figure 1. The dependence of volume upon the tensile stress, and a comparison between our general relation and each of Murnaghams EOS, Birch-Murnaghams EOS and Vinet EOS, for: (a) C; (b) Si; (c) Ge; and (d) α -Sn.

$$P_V = 3B_o \left[1 - \left(\frac{V}{V_o} \right)^{\frac{1}{3}} \right] \left[\left(\frac{V}{V_o} \right)^{-\frac{2}{3}} \exp \left\{ \frac{3}{2} (B'_o - 1) \left[1 - \left(\frac{V}{V_o} \right)^{\frac{1}{3}} \right] \right\} \right] \quad (10)$$

To get a wide understanding of the four elements properties, the microhardness (H) [36] and the Young modulus (E) [37] are also calculated as below:

$$H = (\zeta)^2 \frac{P_T}{3(1-\zeta)} \quad (11)$$

$$E = \frac{P_T}{\varepsilon} \quad (12)$$

where ζ is (a/a_o) and ε is the strain. Also the speed of sound (v_s) is calculated as [29]:

$$v_s \approx \sqrt{\left(v_{os}^2 + \frac{B'_o P_T}{\rho_o} \right) \exp(-\varphi)} \quad (13)$$

where ρ_o and v_{os} are the density and the velocity of sound at [z-PT], respectively. The velocity of sound equals the average of phonons velocity (\bar{v}_{ph}) [38]. And from [30], the phonon velocity, angular frequency (\bar{w}_{ph}), phonon energy (\bar{E}_{ph}) and the plasmon energy (E_{pl}) equal:

$$\bar{v}_{ph} = v_s \quad (14)$$

$$\bar{w}_{ph} = \left(\frac{6\pi^2 N}{V} \right)^{\frac{1}{3}} v_s \quad (15)$$

$$\bar{E}_{ph} = \hbar \bar{w}_{ph} \quad (16)$$

$$E_{pl} = \hbar \sqrt{\frac{n_e e^2}{\varepsilon_o m}} \quad (17)$$

where n_e is the volume of the bond which equals [39]:

$$n_e = \frac{3\sqrt{3}}{2d^3} \quad (18)$$

and N is the number of atoms in the unit cell which equals 8, e and m are the charge and the mass of electron respectively, and ε_o is the permittivity of vacuum. By gathering Equations (15), (16) and (6), one can get:

$$\bar{E}_{ph} (eV) = \frac{\hbar k}{e} \sqrt{v_{so}^2 + \frac{B'_o P_T}{\rho_o}} \exp\left(-\frac{\varphi}{6}\right) \quad (19)$$

$$k \equiv \sqrt[3]{\frac{6\pi^2 N}{V_o}} \quad (20)$$

Gathering Equations (17), (18) and (6), one can get:

$$E_{pl} (eV) = 210.0563 \sqrt{\frac{\exp(\varphi)}{V_o}} \quad (21)$$

3. Results and Discussion

The results of the present work illustrated in **Table 2**, are in good agreement with experimental results of bulk materials. So we can assume that the structural properties of 216 atom clusters (1.21 nm, 4.32 nm, 4.89 nm, and 7.35 nm for C, Si, Ge, and Sn respectively) are properties of the corresponding bulk materials.

As shown in **Figures 2** and **3**, the increase of tensile stress leads to an increase of volume and a decrease in the density. Strain, caused by tensile stress, gives the following results:

1) Alterations of the orbitals [39], and an increase of the distance between atoms [40].

2) A decrease of the bond strength [41] which depends on the distance [42].

3) A decrease of the bulk modulus [43]. It is known that the bulk modulus represents the resistance of matter to the change in volume [44], and it can be considered as the sum of the bulk modulus of all atoms [45] according to the AIM (atoms in molecules) theory [46]. Because the bulk modulus depends directly upon the density [47] and the charge distribution between atoms [48,49], *i.e.* the bonds [44], the bulk modulus decreases with the tensile stress.

4) A decrease of the Young modulus because it depends upon the bulk modulus [47].

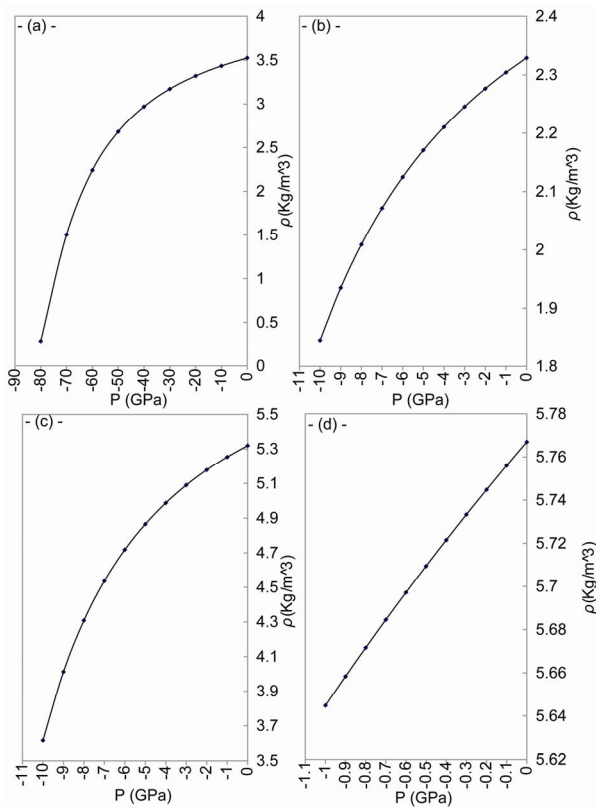


Figure 2. The change of density with tensile stress for: (a) C; (b) Si; (c) Ge; and (d) α -Sn.

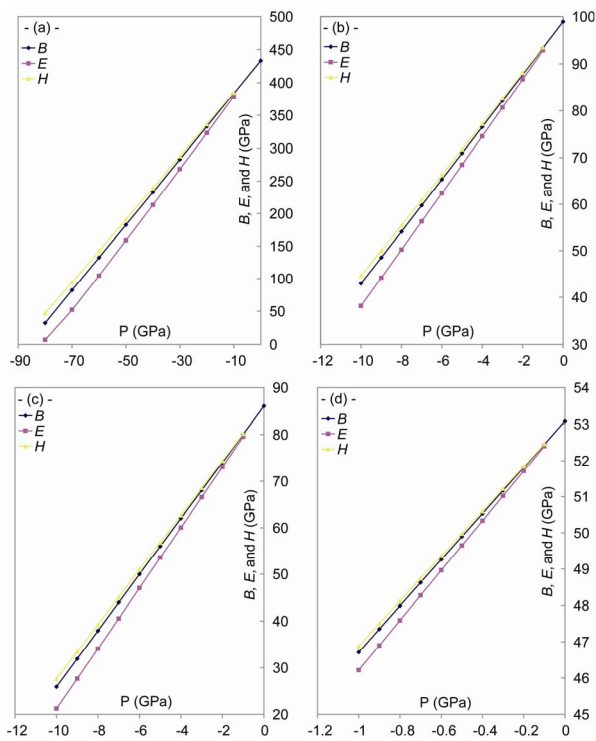


Figure 3. Effect of the tensile stress on the bulk modulus, Young's modulus and the microhardness for: (a) C; (b) Si; (c) Gr; and (d) α -Sn.

5) An increase of the rigidity because the tensile stress decreases the microhardness [50].

As shown in **Figures 4-6**, the speed of sound, the energy of phonon and the energy of plasmon decrease when the tensile stress increases.

The sound waves produce charge distribution, according to Kornushin who has showed that the plasma affects the charge distribution and so the sound wave [51]. On the other hand, the phonon frequency affects the effective charge [52], because the effective charge depends upon the charge distribution and determines the plasma frequency [53]. According to Sanjurjo, the compressive pressure increases the effective charge for IV-IV materials and vice versa [52]. Meanwhile, depending on Burstein who has illustrated that the decrease in the effective charge decreases the plasmon frequency [53], one can find that our results of the behavior are in good agreement with experiment [52] for both the plasmon and phonon energies.

It is shown from **Figure 7** that the vibrational energy increases as the tensile stress increases. Many properties of solids depend on the phonons which determine the atoms vibration [54], where the velocity of sound depends on the atoms arrangement [55]. The crystal is considered as a group of harmonic oscillators [56], according to Born-von Kármán theory, in order that the atoms in the lattice

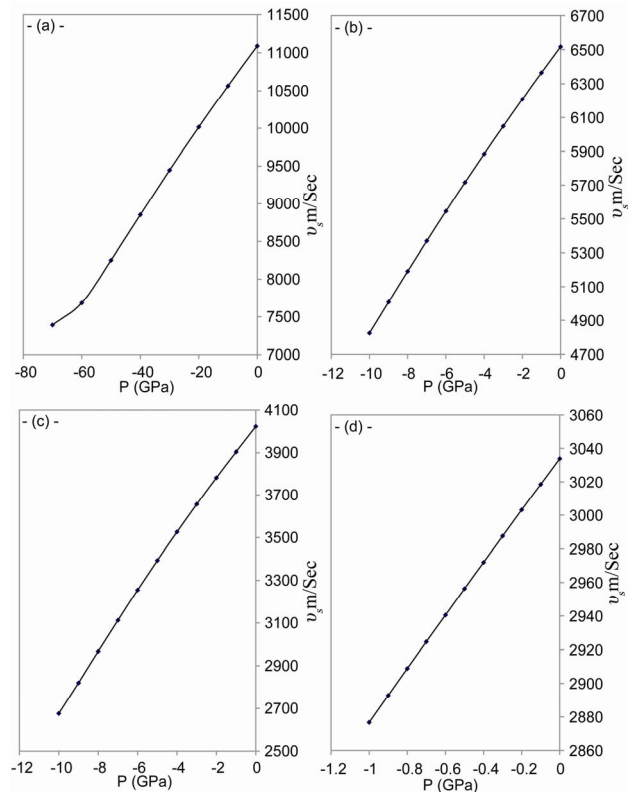


Figure 4. The change of speed of sound with tensile stress for: (a) C; (b) Si; (c) Gr; and (d) α -Sn.

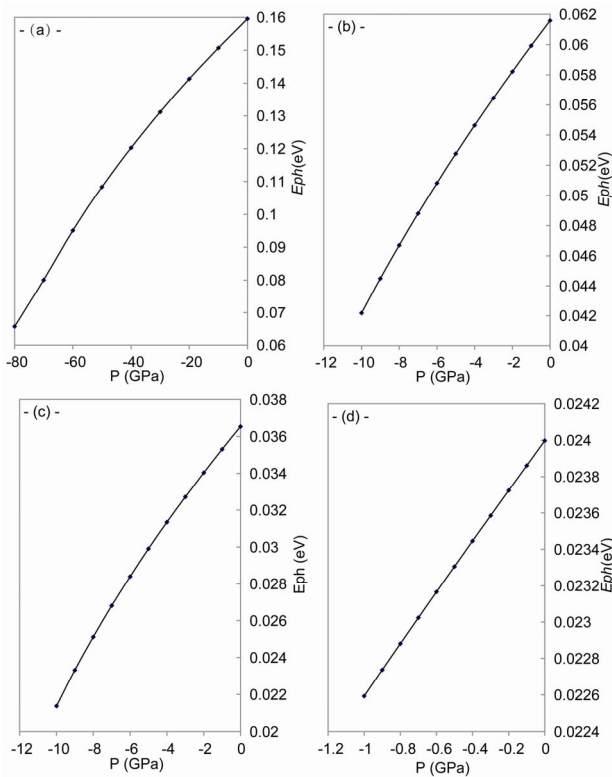


Figure 5. The change of speed of sound with tensile stress for: (a) C; (b) Si; (c) Gr; and (d) α -Sn.

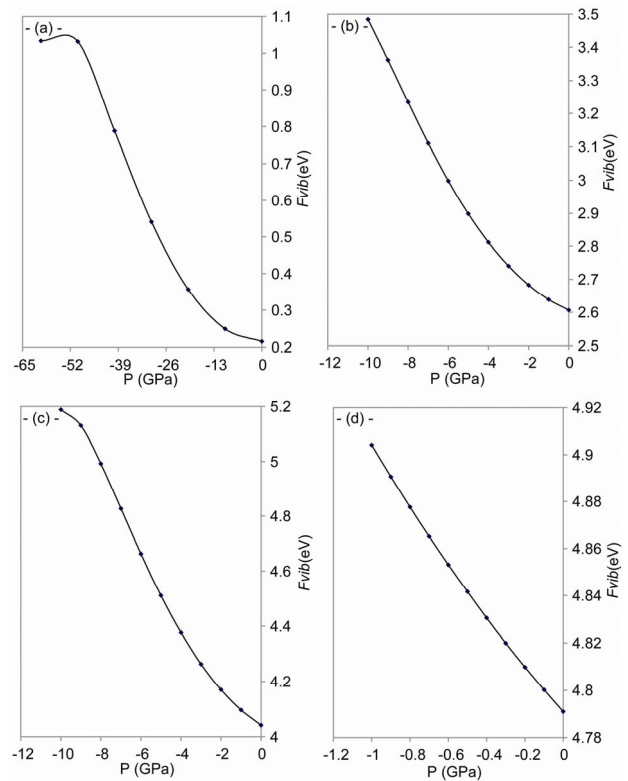


Figure 7. Effect of tensile stress on the vibrational energy for: (a) C; (b) Si; (c) Gr; and (d) α -Sn.

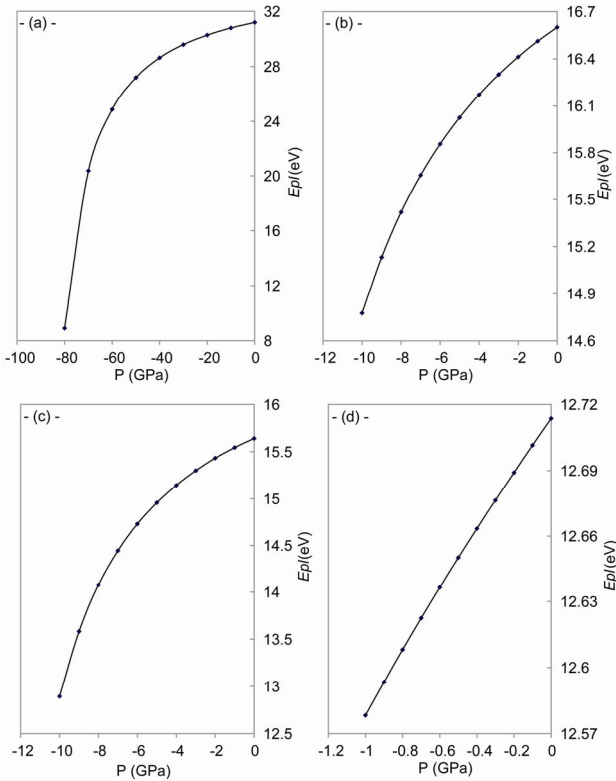


Figure 6. The change of plasmon energy with tensile stress for: (a) C; (b) Si; (c) Gr; and (d) α -Sn.

interplay with the nearest atoms only [57]. From all above and according to Polit who mentioned that the change of the lattice constant changes the charge distribution which affects the atoms' force field and these potentials modify the vibration energy [58].

4. Conclusions

From the results of the present work, it can be concluded that:

- 1) The 216 atom clusters of C, Si, Ge, and α -Sn can be considered as bulk materials concerning the structural properties.
- 2) The range of the elastic deformation for diamond is the smallest.
- 3) The higher the tensile stress, the higher the rigidity of the sample.
- 4) The inclusion of the bulk modulus in every change may be very important in some properties because it can limit their variation range caused by external factors.
- 5) The relation of phonons gives approximated results, however, it is simple and could be used for behavior study.

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