

# **The correlation between some structural properties of IV materials with compression stress**

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## **Abstract**

Lattice constant, density, total energy, cohesive energy, bulk modulus, microhardness, Young modulus, speed of sound, energy of acoustic phonons, plasmon energy and vibrational energy, for diamond, silicon, germanium, and gray tin, all have been calculated and studied when compression stress is exerted. It is found that most of them increase with pressure except the lattice constant which decreases and the vibrational energy behaves in different ways depending upon the matter. The bulk modulus is suggested to correlate to the lattice constant in every change with pressure and it had been regarded in all other properties' calculations. This correlation is used as simple formula as well as new simple formula had been suggested for plasmon-pressure relation.

## **I. Introduction**

Diamond (C) silicon (Si), germanium (Ge) and grey tin ( $\alpha$ -Sn) all have diamond structure, eight atoms per unit cell, four covalent bonds,  $sp^3$  [Myles *et al.* 2001] valence shell and 6, 14, 32 and 50 atomic number respectively [Kittle 1996]. These general properties [Cataldo 2001] of the semiconductors make them used in many fields [Gaith and Alhayek 2009] such as electronics [Gabrysch 2008]. Many researcher have studied their structure such as [Stallcup *et al.* 1996]. The novel here is two things, the change of the bulk modulus versus pressure which had been regarded in every variation of the other properties with pressure, is the first point and the second point is the simple relations of these variations. Although one of them, which is the variation of sound with pressure, was very approximated but in general it could be used to study the behavior of the atoms under pressure, which is very interesting field [Sun 2007]. The aim of this paper is to study the mechanical properties which are regarded as very interested field [Shokrieh and Rafiee 2010].

The CNDO/2 method with STO (Slater Type Orbital) and LCAO (Linear Combination of Atomic Orbitals) approximation were used for calculating the lattice constants, cohesive energy and total energy and as a result of that bulk modulus, Young modulus, microhardness, speed of sound, the energy of phonons and the plasmon energy all have been determined. In the meanwhile the change of the bulk modulus when volume changes with respect to pressure was being both suggested and included in all other calculations such as strain, speed of sound, etc.

## **III. Results and discussion**

Our calculated structural properties compared with other results are shown in table (2).

### **III. 1. Volume and hardness**

As shown in figure (1) that the increase in pressure leads to a decrease in volume and an increase in the density because the orbitals shrink [Connerade *et al.* 2000] and it decreases the distance between atoms [Sze 1990], which entails an increase in bond strength [Jiang *et al.* 2002] which increases the bulk modulus [D'Evelyn and Taniguchi 1998] because it depends upon the density directly [Wang

*et al.* 2010] and it represents the resistance of matter to the change in volume [Mattesini and Matar 2001] and composes of the sum of the bulk modulus of each atom [Pendás *et al.* 2000] according to the theory of atoms in molecules (AIM) [Pendás 2002]. Also the microhardness increases with the increase of pressure because the increase in the rigidity [Yu *et al.* 2010] as well as the Young modulus which depends upon the bulk modulus [Wang *et al.* 2010] while the minus sign refers to the compression stress because all them are controlled by the bond strength [D'Evelyn and Taniguchi 1998].

The change in bulk modulus had been included in every change in pressure that why our curve  $P-V/V$  has a wide convergence from the other equations of state which is illustrated in figure (2).

### III. 2. Energy of phonon and plasmon

As shown in figures (4 and 5), the speed and the energy of sound and the energy of plasma increase when pressure is increased.

The sound waves produce charge distribution, according to Kornysushin who shows that the plasma affects the charge distribution and so the sound wave [Miranda and Haar 1972], on the other hand the phonon frequency affects the effective charge [Sanjurjo *et al.* 1983], because the effective charge depends upon the charge distribution and determines the plasma frequency [Burstein *et al.* 1968]. According to Sanjurjo, the pressure increases the effective charge for IV-IV materials [Sanjurjo *et al.* 1983], and Burstein had mentioned that the increase in the effective charge increases the plasmon frequency [Burstein *et al.* 1968], so our results of the behavior are in good agreement with experiment [Sanjurjo *et al.* 1983] for both plasma and phonon energies.

### III. 3. Vibrational energy

Figure (6) shows a variance in results, the diamond vibrational energy increases, but that of grey tin decreases, while both silicon and germanium show a similar behavior but different from the two other because the vibrational energy of them shows a decrease and an increase.

Many properties of solids depend on the phonons which determines the atoms vibration [Parliński 2005] in the meanwhile the velocity of sound depends on the atoms arrangement [Iitaka and Ebisuzaki 2001] so and because the crystal is considered as a group of harmonic oscillators [Xie *et al.* 1999] according to Born-von Kármán theory, so the atoms in the lattice were represented as a mainspring [Wang *et al.* 2006] which interplay just with its nearest atom [Malinowska-Adamska *et al.* 2006] so we believe that this variant behavior can be mainly attributed to the bond properties of each matter such as bulk modulus which mainly depends on charge distribution between atoms [Fernandez *et al.* 2004], cohesive energy which reflects the bond strength [Sun 2007], bond length, etc. as shown in Figure (7).

## IV. Conclusions

1. The heat spreads faster when a load is applied to the sample.
2. Under pressure or load the sample, especially the electronic devices, may be ruined more than other which do not encounter loads such as bags, hands etc.
3. Infrared absorption increases with pressure [Burstein *et al.* 1968].

4. In general our results and relations can be used with high agreement in calculations and behavior.