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Evaluating of Some Elastic Properties for Nanosemiconductors Under High Pressure

Siham J. AL-Faris[1], Raghda Tareeq Abdulateef[2], Hamssa B. Mohammed[3], and Raed Hashim AL-Saqa[4]

[1]*College of Education for Pure Science, Department of Physics, University of Al-Hamdaniya, Al-Hamdaniya, Iraq*
[2]*College of Medicine, University of Mosul, Mosul, Iraq*
[3]*Science College, Techniques Department, University of Mosul, Mosul Iraq*
[4]*Directorate General of Education, Ministry of Education, Nineveh, Iraq*

Elastic properties for some nanosemiconductors, such as bulk modulus (B) and volume expansion (V/V_0) for CdSe (4.2 nm), γ-Al_2O_3 (67 nm), γ-Al_2O_3 (37 nm), CeO_2 (cubic fluorite, 15 nm), CeO_2 (orthorhombic phase, 15 nm), CuO (24 nm), and TiO_2 (rutile, 10 nm), are studied under high pressure to predict the effect of pressure on them, using two equations of state (EOS), *viz.*, Bardeen's and Thomsen's EOS, and compared them with experimental results from literature. The study proves that the Bardeen's EOS is more suitable and in agreement for given nanoscale semiconductors than the Thomsen's EOS.

Пружні властивості деяких нанонапівпровідників, такі як модуль об'ємної пружности (B) й об'ємне розширення (V/V_0) для CdSe (4,2 нм), γ-Al_2O_3 (67 нм), γ-Al_2O_3 (37 нм), CeO_2 (кубічний флюорит, 15 нм), CeO_2 (орторомбічна фаза, 15 нм), CuO (24 нм) і TiO_2 (рутил, 10 нм), було досліджено під високим тиском для прогнозування впливу тиску на них за допомогою двох рівнянь стану, а саме, Бардінового та Томсенового рівнянь стану, та порівняно їх з експериментальними результатами з літератури. Дослідження доводить, що Бардінове рівняння стану є більш придатним та узгодженим для заданих нанорозмірних напівпро-

відників, аніж Томсенове рівняння стану.

Key words: nanosemiconductors, equation of state, Bardeen's equation, Thomsen's equation, elastic properties, γ-Al_2O_3, CeO_2, CuO, TiO_2, CdSe.

Ключові слова: нанонапівпровідники, рівняння стану, Бардінове рівняння, Томсенове рівняння, пружні властивості, γ-Al_2O_3, CeO_2, CuO, TiO_2, CdSe.

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1. INTRODUCTION

The studying of nanoscale semiconductor materials with dimensions smaller than 100 nm is a popular topic in chemistry, physics, and engineering [1]. As well known, applying high pressure to a substance can effectively affect its crystal and electronic structures [2]. Unlike doping, applying high pressure prevents the introduction of contaminants and allows layered materials to reveal their intrinsic capabilities [3]. Miguel [4] conducted a rigorous analysis of the projected impacts and benefits of pressure on nanomaterials. High pressure on nanoparticles causes a variety of phenomena, including ionization and changes in electrical characteristics under pressure. As a result, the volume–pressure and bulk-modulus relationship of condensed material, which represents the equation of state, is a fundamental concept. Despite the fact that there are numerous equations of state (EOS) in the literature, the pressure effect at constant temperature on nanomaterials remains unknown. For example, the commercial world has been very interested in lithium–aluminium–silicate ceramics due to their low thermal expansion, strength, transparency, and chemical robustness. As a result, research into the changes of nanosize materials according to high pressure is critical, particularly, given the enormous potential for applications using nanoscale materials. Several experiments were conducted to examine and explain the behaviour of nanomaterials [5, 6].

The EOS recently developed for nanosemiconductors are critically examined. The several conceivable kinds of EOS are described, along with their relationships. For this purpose, we considered seven types of nanosemiconductors, *viz.*, CdSe (4.2 nm), Fe_2O_3 (10 nm), γ-Al_2O_3 (67 nm and 37 nm), CeO_2 (cubic fluorite, 15 nm), CeO_2 (orthorhombic, 15 nm), CuO (24 nm), TiO_2 (rutile, 10 nm) (and TiO_2 (anatase, 40 nm)). Both the results and the available experimental data are in a good accord. The recently developed EOS for nanomaterials are directly evaluated. The various versions of the EOS are described, along with their relationships. The above-mentioned semi-

conductor nanomaterials were chosen because they are widely used in solar-cell applications and different electronic devices.

2. METHOD OF ANALYSIS

2.1. Bardeen's EOS

Bardeen relied on the compressibility of materials, using the theory of interatomic potentials to understand the ability of a material to reduce the interatomic distances and with the help of the Grüneisen approximation to describe compressibility and the coefficient of volume expansion and its derivative at constant temperature, where the Bardeen equation can be used in the following form [7]:

$$P_B = 3B_0\left[\left(\frac{V}{V_0}\right)^{-5/3} - \left(\frac{V}{V_0}\right)^{-4/3}\right]\left[1+\frac{3}{2}\left(B_0'-3\right)\left(\left(\frac{V}{V_0}\right)^{-1/3}-1\right)\right]. \quad (1)$$

2.2. Thomsen's EOS

The Thomsen's equation of state is a thermodynamic relationship between the isothermal compressibility, the density, and the bulk modulus that can be derived from the Helmholtz free energy. The modern version of the Thomsen's equation of state was developed by industry and used in the analysis of seismic data. Nevertheless, the roots of the equation should lie in previously established hydrostatic-gas law. The Thomsen's equation of state relates the isothermal bulk modulus to the density and its intrinsic derivative, the isothermal compressibility. In practical applications, the Thomsen's equation has been used primarily as a quadratic three-parameter equation fitting seismic data from oil exploration. However, to develop a theoretical understanding of the Thomsen's equation, a theoretical expansion is used to calculate the second order in the density and the third order in the internal energy, using the following form of the equation [8]:

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

2.3. Volume Expansion

The availability of experimental data is the reason we chose these

materials: CdSe (4.2 nm), γ-Al_2O_3 (67 nm and 37 nm), CeO_2 (cubic fluorite, 15 nm), CeO_2 (orthorhombic, 15 nm), TiO_2 (rutile, 10 nm), and CuO (24 nm). Table lists the necessary input data. The Bardeen's and Thomsen's equations of state were used to calculate the volume expansion and bulk modulus for nanomaterials at various pressure values up to approximately 50 GPa. The results can be seen in Figs. 1–6. These results were an approach to the experimental results of the literature used at low pressures (less than 30 GPa), but they diverged slightly at high-pressure values (more than 30 and up to 50 GPa).

Data on (V/V_0) have been evaluated using Eq. (1) and (2), respectively, for given nanosemiconductors. Outcomes are displayed in figures and contrasted with data from experiments. We may be neglecting higher-order factors in Eqs. (1) and (2) as a result of the deviation from experimental values at high pressures. For comparison sake, Figs. 1–3 display the findings along with the pertinent experimental data [4–6].

TABLE. Bulk modulus and its derivative at ambient pressure

Nanosemiconductors	B_0, GPa	B_0'	Refs.
CdSe (4.2 nm)	74	4	7
CeO_2 (cubic fluorite phase, 15 nm)	328	4	12
CeO_2 (orthorhombic phase, 15 nm)	326	4	13
γ-Al_2O_3 (67 nm)	238	4	14
γ-Al_2O_3 (37 nm)	172	4	15
CuO (24 nm)	81	4	16
TiO_2 (rutile phase, 10 nm)	211	4	17–18

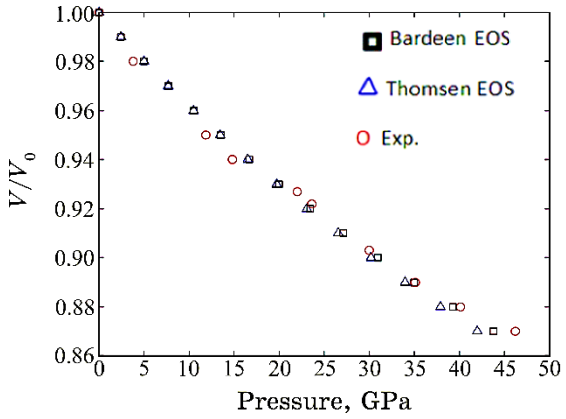

Fig. 1. Variation of (V/V_0) *via* pressure for γ-Al_2O_3 (67 nm).

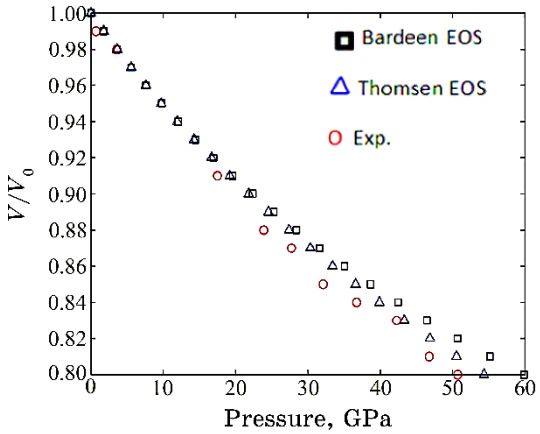

Fig. 2. Variation of (V/V_0) *via* pressure for γ-Al_2O_3 (37 nm).

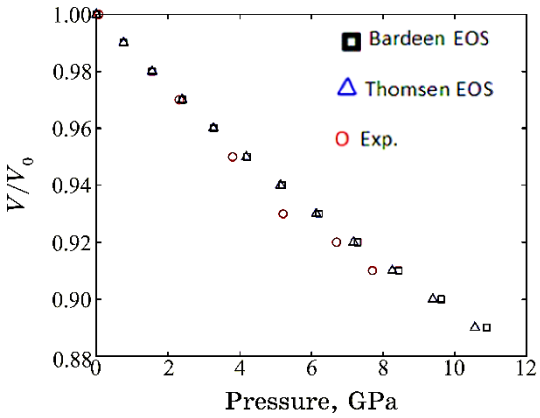

Fig. 3. Variation of (V/V_0) *via* pressure for CdSe (4.2 nm).

At low pressure, the results of Eqs. (1) and (2) are shown to be in a good agreement with the experimental data; nevertheless, at high pressure, they diverge. Given the pressure range under consideration, it may be said that Eqs. (1) and (2) are more than enough for these materials. This demonstrates unequivocally the justification of the approximation employed in Eqs. (1) and (2). It should be noted that, at low pressures, all of the equations of state (Thomsen's and Bardeen's ones), which were covered in this paper, matched the actual results.

A good agreement between the theoretical values of V/V_0, obtained from Eqs. (1) and (2), was also found with the corresponding experimental data for given nanoscale, especially, at low pressures (less than 35 GPa) compared to other EOS for a large range of na-

noscale semiconductors.

2.4. Bulk Modulus

Studying equations of state has the benefit of being correlated with bulk modulus (B), which allows us to determine the pressure dependence of the latter. The pressure that causes a relative change (reduction) in a material volume is known as the bulk modulus and can be expressed mathematically as [9]

$$B = -\frac{\Delta P}{\frac{\Delta V}{V}}. \tag{3}$$

The form of Eq. (3) is obtained by rearranging this equation:

$$B = -V\frac{dP}{dV}. \tag{4}$$

In addition to showing that the bulk modulus rises with rising pressure or a decrease in the volume of the solid-material unit cell, Eq. (4) depicts the bulk modulus as a function of pressure. Experiments have demonstrated that the bulk modulus is dependent on the compression generated in the material at a specific temperature. Strong repulsive interatomic forces are created against the external agent, when the lattice gap is reduced due to high pressure [10, 11]. Therefore, Eq. (4) is used to obtain the bulk modulus comparable to each EOS.

The Bardeen's and Thomsen EOS are derived with respect to volume in order to produce the following equations, which are used to determine the bulk modulus at high pressure:

$$B_B = B_0\left[9\left(B_0'-3\right)\left(\frac{V}{V_0}\right)^{-2} - 5\left(3\left(B_0'-3\right)-1\right)\left(\frac{V}{V_0}\right)^{-5/3} - \right.$$
$$\left. -4\left(1-\frac{3}{2}\left(B_0'-3\right)\right)\left(\frac{V}{V_0}\right)^{-4/3}\right], \tag{5}$$

$$B_{Th} = \frac{B_0}{2}\left[-\left(\frac{3}{2}B_0+1\right)\left(\frac{V}{V_0}\right)^{1/3} - \left(1-\frac{3}{4}B_0'\right)\left(\frac{V}{V_0}\right)^{-1/3} + \frac{9}{4}B_0'\left(\frac{V}{V_0}\right)\right]. \tag{6}$$

The above two equations give the change in the bulk modulus with the change in the pressure applied to the solid-state materials (Figs. 4–6).

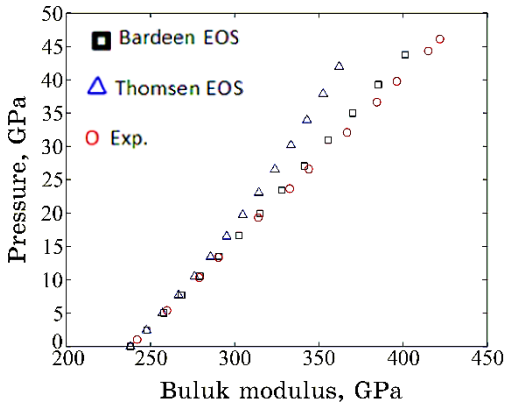

Fig. 4. Variation of bulk modulus *via* pressure for γ-Al_2O_3 (67 nm).

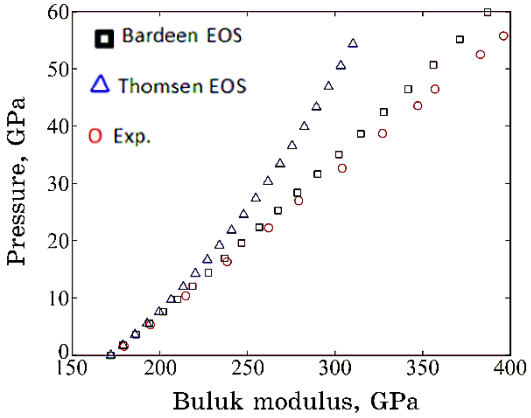

Fig. 5. Variation of bulk modulus *via* pressure for γ-Al_2O_3 (37 nm).

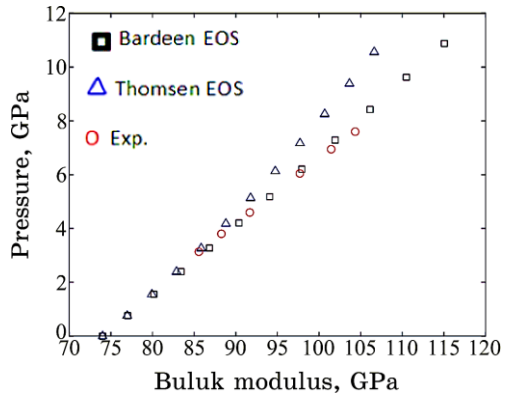

Fig. 6. Variation of bulk modulus *via* pressure of CdSe (4.2 nm).

6. CONCLUSION

The volumetric expansion and bulk modulus as a function of pressure were studied for some different nanosemiconductors (CdSe (4.2 nm), γ-Al_2O_3 (37 nm and 67 nm), CeO_2 (orthorhombic, 15 nm), CeO_2 (cubic fluorite, 15 nm), CuO (24 nm), and TiO_2 (rutile, 10 nm). Obtained results agree well with the available experimental data, especially, at low pressures (less than 35 GPa), but, when the pressure increased to 50 GPa, we found a deviation in the results, as the results of the Bardeen's equation were closer in comparison with the results of the Thomsen's equation that indicates that the Bardeen's equation is closer to the experimental results and, therefore, can be used over a wide range of pressure values to study the physical properties of nanosemiconductors under high pressures, especially, at pressure values, which are difficult to reach experimentally.

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