International Journal of Computational Research and Development (IJCRD)
Impact Factor: 5.015, ISSN (Online): 2456 - 3137
(www.dvpublication.com) Volume 8, Issue 2, 2023

EFFECT OF HIGH PRESSURE ON STRUCTURAL AND THERMO ELASTIC PROPERTIES OF SEMICONDUCTORS

Chandra Kumar Dixit
Post Doctoral Research Scholar, University of Marlyne, International Coordinate Office, Overland Park, Kansas, United States of America

Cite This Article: Chandra Kumar Dixit, "Effect of High Pressure on Structural and Thermo Elastic Properties of Semiconductors", International Journal of Computational Research and Development, Volume 8, Issue 2, July - December, Page Number 22-31, 2023.

Abstract:

In this paper, we have theoretically predicted the structural and thermoelastic properties of certain semiconductors using equations of state. The calculations have been performed on semiconductors (ZnS, ZnSe, ZnTe) with a cubic zinc-blende (ZB) structure. Various properties such as lattice constant, bulk modulus, first derivative of bulk modulus, volume compression ratio (V/V0), relative isothermal expansion coefficient (α), and Gruneisen Parameter have been determined using different equations of states (EOSs). We observed that, with increasing pressure, the volume decreases, bulk modulus increases, the first pressure derivative of bulk modulus decreases, Gruneisen parameter decreases, lattice parameter decreases, and the relative isothermal expansion coefficient (α) decreases for ZnS, ZnSe, and ZnTe semiconductors.

Key Words: EOS, Lattice parameter, Gruneisen Parameter, Bulk Modulus, Semiconductors, Volume Compression Ratio.

Introduction:

Semiconductors have become a very hot topic for researchers due to their revolutionary technological applications in numerous areas. Considering the significant amount of work done by researchers in developing semiconductor technology, the effect of pressure on these materials has been taken into consideration. Most semiconductors have a structure consisting of a number of covalent bonds, giving them a net-like structure. This type of structure leads to an open crystal structure, similar to how water becomes denser upon melting. High-pressure researchers find semiconductors intriguing because they exhibit a series of high-pressure phase transitions to denser structures. Studying the effect of high pressure on semiconductors is an interesting research field within material science, similar to the exploration of materials below 20 K by low-temperature specialists. Conducting research on semiconductors at high pressure is challenging, as researchers must produce, apply, and measure high pressure on the materials while simultaneously observing their physical and chemical properties. This implies that these pressures must be sustained for a sufficiently long time. The field of semiconductors under high pressure is fascinating for several reasons. For example, at high pressure, the bulk modulus increases, volume decreases, pressure derivative of bulk modulus decreases, and the Gruneisen parameter declines [1, 2]. The changes in thermoelastic and mechanical properties of solids at high pressure can lead to the emergence of new materials with useful applications in the modern era. In the present study, three semiconductors (ZnS, ZnSe, ZnTe) with a cubic zinc blende (ZB) structure were considered. Zinc sulfide (ZnS) is an essential semiconductor that has garnered great interest in recent decades due to its applications in science and technology [3]. It is a wide and direct bandgap semiconductor, making it useful for applications in laser diodes, high-density optical memory, solar cells, and electronic image displays [3]. Zinc selenide (ZnSe) exhibits excellent photovoltaic and optical properties and finds applications in thin-film solar cells, nonlinear optical crystals, photoluminescent materials, blue-green light-emitting diodes, lasers, and electroluminescent devices [4,5]. Zinc telluride (ZnTe), also a wide-band-gap semiconductor, is typically found in the cubic zinc-blende structure and shows promise for applications as a purely green light-emitting diode. Understanding the pressure dependence of the elastic properties of a compound is crucial for developing its optical and electrical properties and for better interpreting the solid-state phenomena of the material. In this study, the theoretical prediction of elastic properties for Zinc Sulfide was made using three equations of state (EOSs): Vinet Rydburg EOS, Modified Lenard Jones EOS, and Birch-Murnaghan EOS. The paper presents variations in compression ratio (V/V0), bulk modulus, first-order pressure derivative of bulk modulus, Gruneisen parameter, relative isothermal expansion coefficient, and lattice constant with pressure.

Method of Analysis:

In the current study we have used three different EOSs. These Equations of states (EOSs) are given below:

The Modified Lenard Jones EOS [6]:

The EOS (1) given below is known as Modified Lenard Jones EOS (ML-Jones EOS),

$$P = \left(\frac{K_0}{j}\right)(m)^{-n}\left[m^{-n} - 1\right] \qquad (1)$$

Where $j = \frac{K_0^{'}}{3}$ and $m = \left(\frac{V}{V_0}\right)$

Using the formula $K_T = -V\left(\frac{\partial P}{\partial V}\right)_T$ Isothermal Bulk modulus can be found by equation (1) as given below:

$$K_T = K_0 m^{-j}[2m^{-j} - 1] \quad (2)$$

First order pressure derivative of Bulk Modulus ($K_T^{'}$) can be obtained by equation $K_T^{'} = \left(\frac{\partial K_T}{\partial P}\right)_T$

$$K_T^{'} = n\left[\frac{-4m^{-j}+1}{-2m^{-j}+1}\right] \quad (3)$$

Vinet - Rydburg EOS [7, 8]:

Equation (4) is known as the Vinet - Rydburg EOS and is given below:

$$P = 3K_0 w^{-2}(1-w)\exp[\eta(1-w)] \quad (4)$$

Where $w = \left(\frac{V}{V_0}\right)^{\frac{1}{3}}$ and $\eta = \frac{3}{2}(K'_0 - 1)$

Isothermal Bulk modulus can be found by equation (7) using the formula

$K_T = -V\left(\frac{\partial P}{\partial V}\right)_T$ $K_T = K_0 \exp\{\eta(1-w)\}w^{-2}[1+(1-w)(\eta w+1)]$ (5)

First derivative of Bulk Modulus ($K_T^{'}$) can be obtained by equation

$K_T^{'} = \left(\frac{\partial K_T}{\partial P}\right)_T$ $K_T^{'} = \frac{1}{3}\left[\frac{x(1-\eta)+2\eta w^2}{1+(1+\eta w)(1-w)} + \eta w + 2\right]$ (6)

Birch - Murnaghan (3rd) EOS [9]:

The Birch - Murnaghan (3rd) EOS have been derived using finite strain theory . Equation (7) is known as Birch- Murnaghan (3rd) EOS.

$$P = \frac{3}{2}[1+\frac{3}{4}(w^{-2}-4)(K_0^{'}-4)]K_0[w^{-7}-w^{-5}] \quad (7)$$

Where $w = \left(\frac{V}{V_0}\right)^{\frac{1}{3}}$

Isothermal Bulk modulus can be found by equation (4) using the formula $K_T = -V\left(\frac{\partial P}{\partial V}\right)_T$

$$K_T = \frac{3}{8}(9w^{-9} - 14w^{-7} + 5w^{-5})K_0(K_0^{'}-4) + \frac{K_0}{2}[7w^{-7} - 5w^{-5}] \quad (8)$$

First order pressure derivative of Bulk Modulus ($K_T^{'}$) can be obtained by equation $K_T^{'} = \left(\frac{\partial K_T}{\partial P}\right)_T$

$$K_T^{'} = \frac{K_0}{8K_T}[(81w^{-9} - 98w^{-7} + 25w^{-5})(K_0^{'}-4) + \frac{4}{3}(49w^{-7} - 25w^{-5})] \quad (9)$$

Relative Isothermal Expansion Coefficient (α_r):

$\alpha_r = \left(\frac{\alpha}{\alpha_0}\right)$, thermal expansion coefficient is the ratio of relative change in volume (V) and change of temperature (T) [10]:

The value of α_r can be calculated as follows:

$$\alpha_r = \left(\frac{K_0}{K_T}\right) \quad (10)$$

Gruneisen Parameter:

The value of Gruneisen parameter (γ) can be calculated by using the formula given by Borton and Stacey [11]:

$$\gamma = \frac{\left(\frac{1}{2}\right)K' - \frac{1}{6} - \frac{f}{3}\left[1 - \frac{1}{3}\left(\frac{P}{K_T}\right)\right]}{1 - \left(\frac{4}{3}\right)\left(\frac{P}{K_T}\right)} \quad (11)$$

Where f=2.35

Lattice Constant:

The effect of pressure on lattice constant can be calculate using the equation given below [12,13]

$$a_p = a_0\left(1 + K_0^{'}\frac{P}{K_0}\right)^{\frac{-1}{3B_0^{'}}} \quad (12)$$

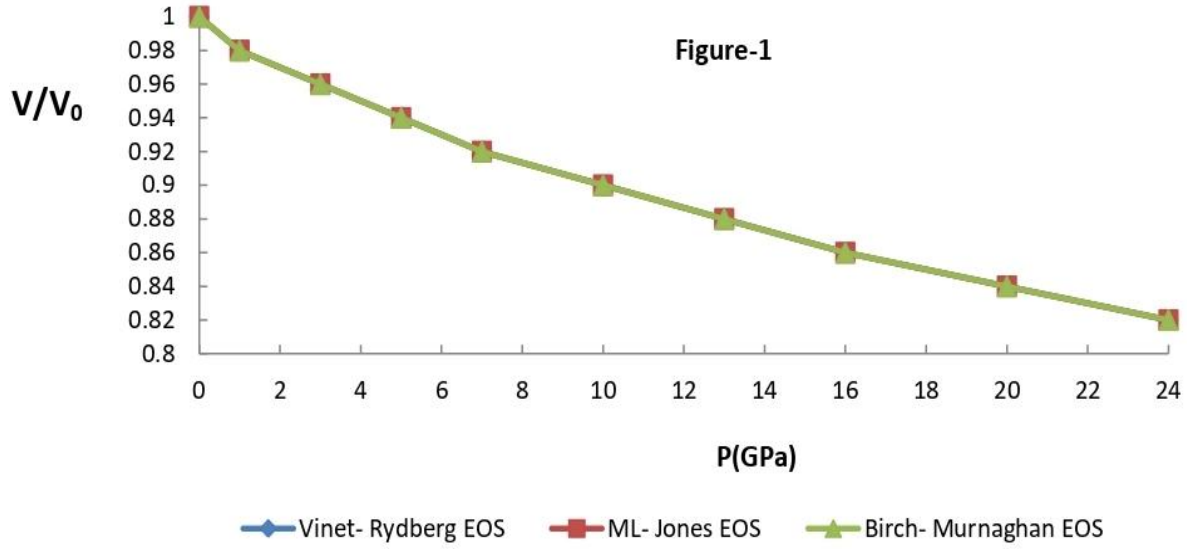
Where a_0 is the lattice parameter at atmospheric pressure, a_p is lattice parameter at pressure P.

Result and Discussion:

The input parameter used in the calculation are given in the following table with references

Semiconductors	K_0(GPa)		$K_0^{'}$		a_0(A^0)	
ZnS	78	[14]	4.54	[15]	5.4102	[16]
ZnSe	59.5	[14]	4.55	[15]	5.668	[17]
ZnTe	50.9	[14]	4.61	[15]	6.101	[18]

Theoretical Prediction of Structural Properties of ZnS:



In figure 1, we observe the graph depicting the relationship between pressure and volume compression ratio (V/V0) for ZnS. Theoretical calculations have been conducted utilizing three distinct EOSs: the Vinet Rydberg EOS, Modified Lenard Jones EOS, and Birch-Murnaghan EOS. Notably, all three EOSs yield remarkably similar results. It is evident that approximately 24GPa pressure is required to compress ZnS to 18% of its original volume. The theoretical graph entirely validates the principle that an increase in pressure leads to a decrease in volume [1, 2].

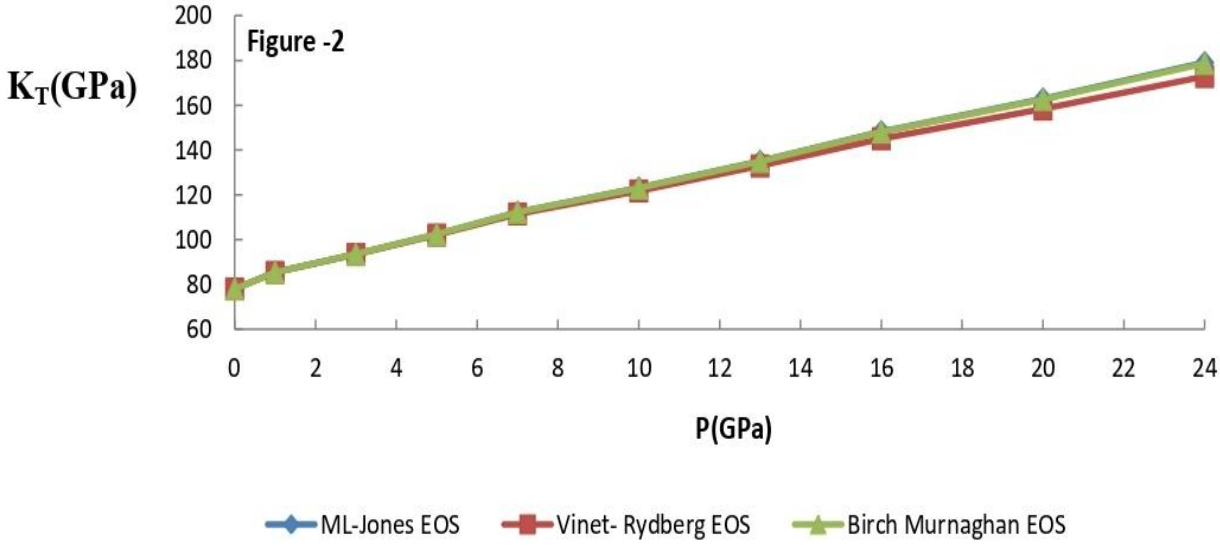


Figure 2 illustrates the relationship between pressure and Bulk modulus (KT) for ZnS. It is evident that as the pressure increases to 24GPa, KT undergoes a significant increment of approximately 125% from its initial value. The calculations were conducted using three distinct equations of state (EOSs): Vinet Rydberg EOS, Modified Lenard Jones EOS, and Birch-Murnaghan EOS. Remarkably, this theoretical graph consistently confirms the principle that an increase in pressure leads to a corresponding rise in volume and Bulk modulus [1, 2].

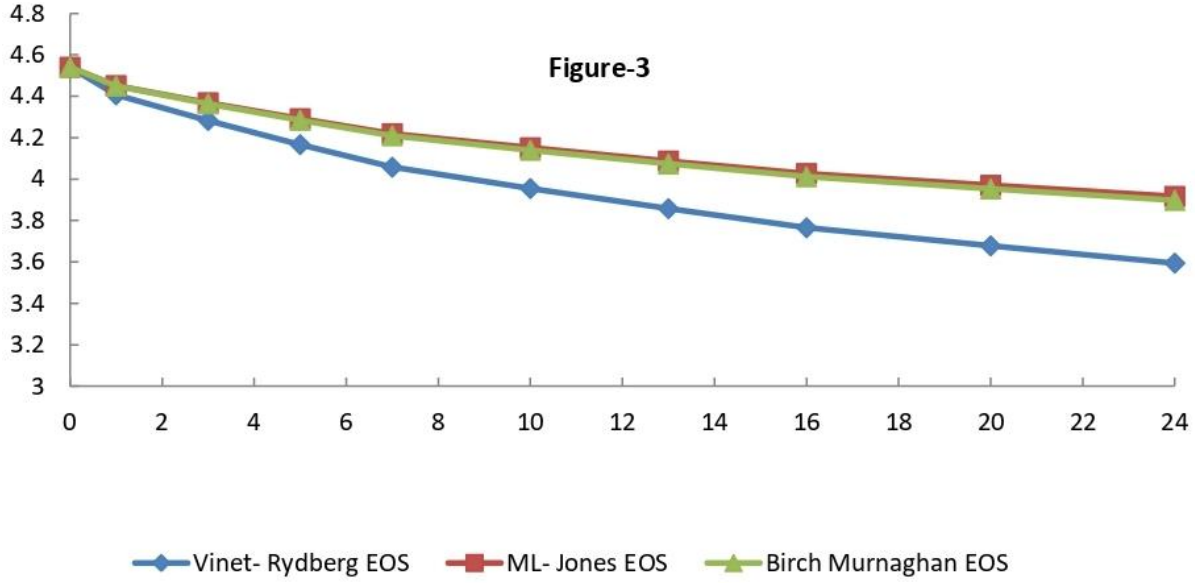


Figure 3 depicts the graph illustrating the relationship between pressure and the first pressure derivative of Bulk modulus for ZnS. It is evident from the graph that decreases continuously as the pressure increases. Furthermore, it is worth noting that the Vinet-Rydberg EOS exhibits some deviation from the other two EOSs (Modified Lenard Jones EOS and Birch-Murnaghan EOS). The theoretical calculation involved the use of three different EOSs (Vinet-Rydberg EOS, Modified Lenard Jones EOS, and Birch-Murnaghan EOS). Remarkably, this theoretical graph perfectly aligns with the established fact that an increase in pressure leads to a decrease in volume [1, 2].

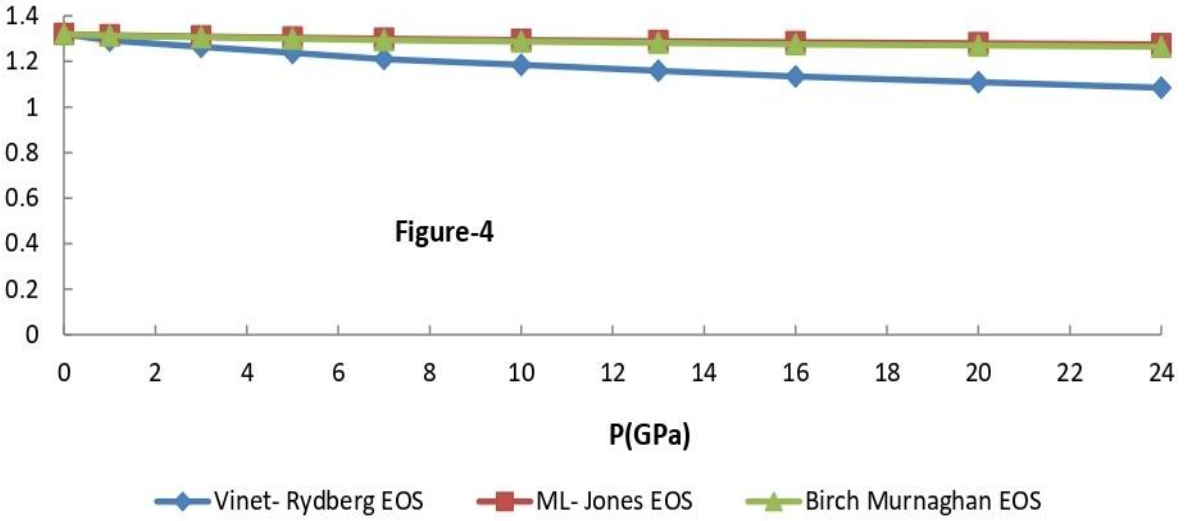


Figure 4 depicts the graph illustrating the relationship between pressure and the Gruneisen parameter for ZnS. Notably, the Gruneisen parameter exhibits a decline as pressure increases. The theoretical calculations were performed using three distinct equations of state (EOSs): the Vinet Rydberg EOS, the Modified Lenard Jones EOS, and the Birch-Murnaghan EOS. Remarkably, this theoretical graph unequivocally corroborates the observation that an increase in pressure leads to a decrease in the volume Gruneisen parameter [1, 2].

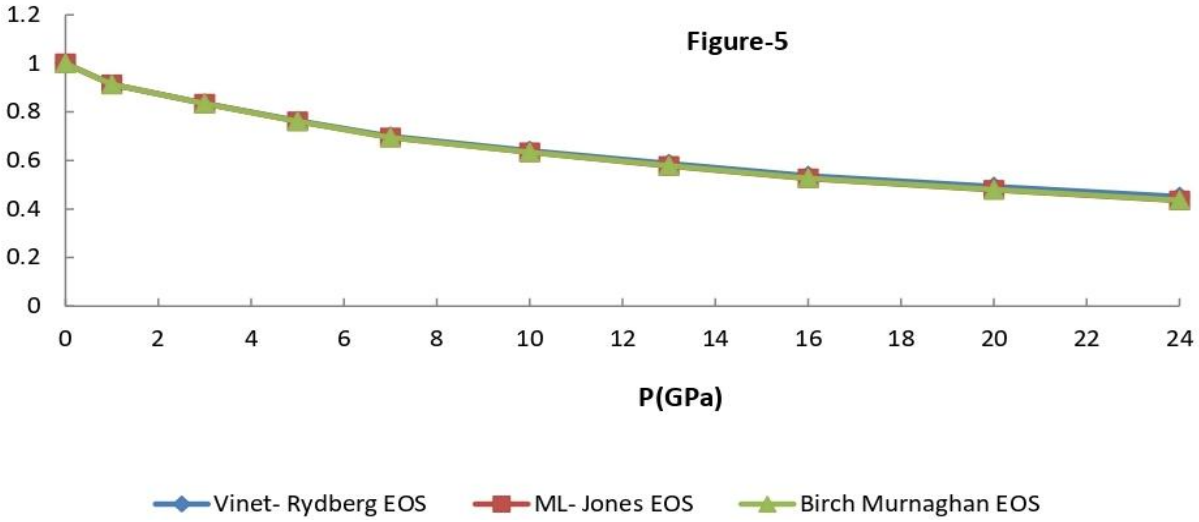


Figure 5 illustrates the graphical relationship between pressure and the Relative Isothermal Expansion Coefficient ( ) for ZnS. It is evident from the graph that declines as pressure increases. Remarkably, the value of diminishes by 57% from its initial state when the pressure rises by 24GPa. Theoretical calculations were conducted using three distinct Equations of State (EOSs): Vinet Rydberg EOS, Modified Lenard Jones EOS, and Birch-Murnaghan EOS. Notably, the results from all three equations coincide precisely, even under high-pressure conditions, as depicted in the aforementioned graph.

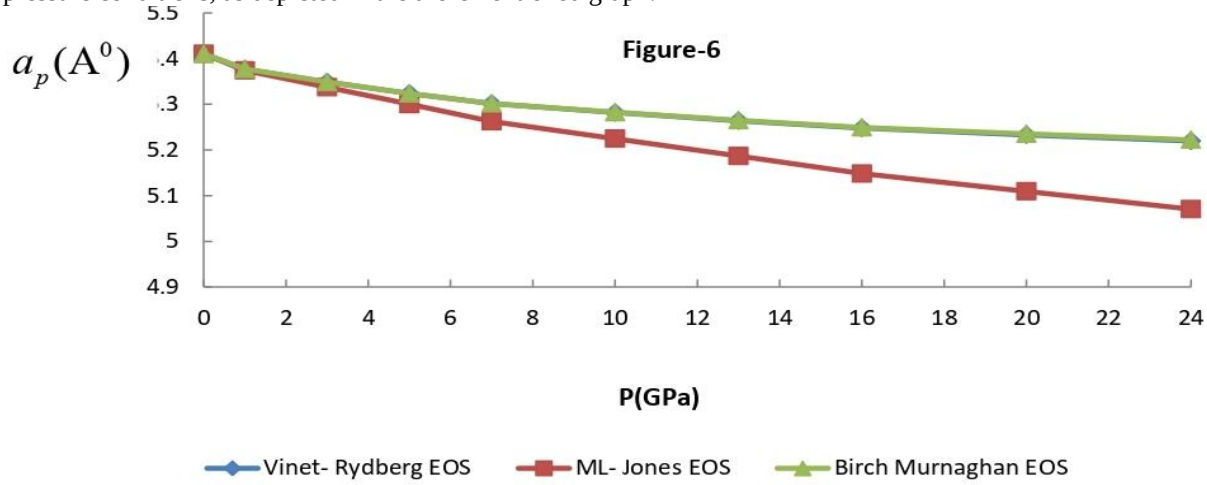
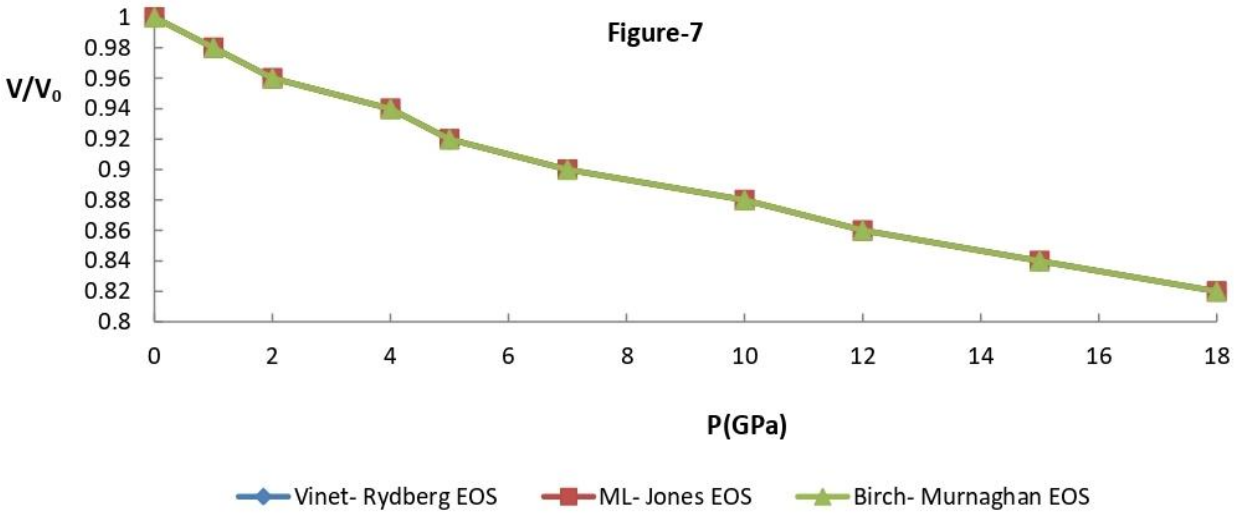
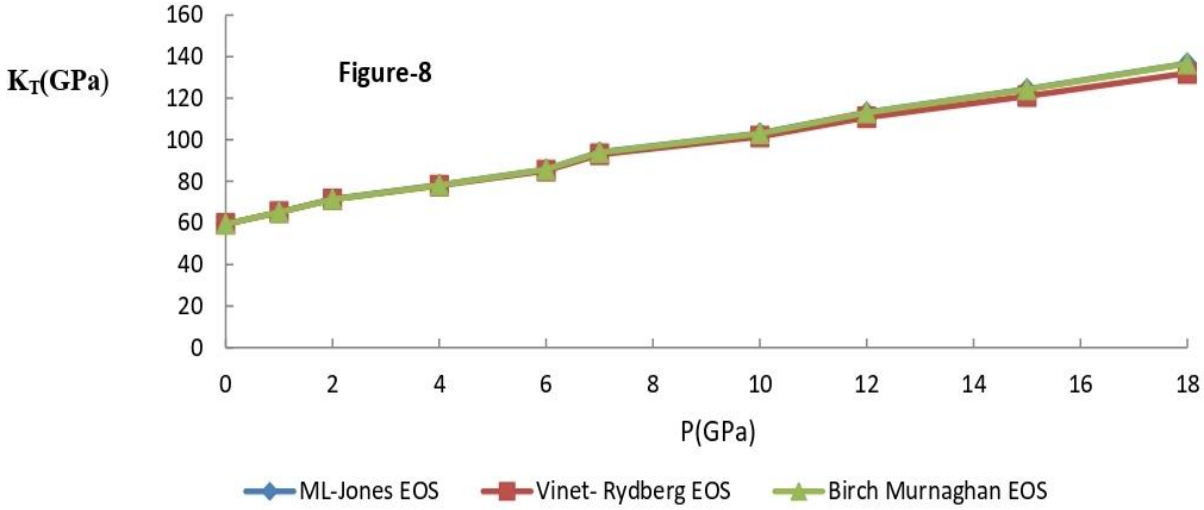


Figure 6 represents the graph between pressure and lattice parameter for ZnS. The theoretical calculation has been made using three different EOSs (Vinet Rydberg EOS, Modified Lenard Jones EOS and Birch- Murnaghan EOS). From this graph we can also notice that lattice parameter decreases at high pressure.

Theoretical Prediction of Structural Properties of ZnSe:



In figure 7, we observe the graphical representation of the pressure and volume compression ratio (V/V0) for ZnSe. Theoretical calculations have been conducted employing three distinct equations of state (EOSs): Vinet Rydberg EOS, Modified Lenard Jones EOS, and Birch-Murnaghan EOS. It is noteworthy that a substantial pressure of approximately 18GPa is required to reduce the volume by 18% from its initial value. Evidently, this theoretical graph consistently corroborates the principle that an increase in pressure leads to a reduction in volume [1 ,2].



In figure 8, we observe the correlation between pressure and Bulk modulus (KT) for ZnSe. Notably, KT demonstrates a remarkable 125% increase from its initial value as the pressure rises to 18GPa. Theoretical calculations have been conducted using three distinct EOSs (Vinet Rydberg EOS, Modified Lenard Jones EOS, and Birch-Murnaghan EOS). The resulting theoretical graph distinctly validates the principle that an increase in pressure leads to a corresponding increase in the volume's Bulk modulus [1,2].

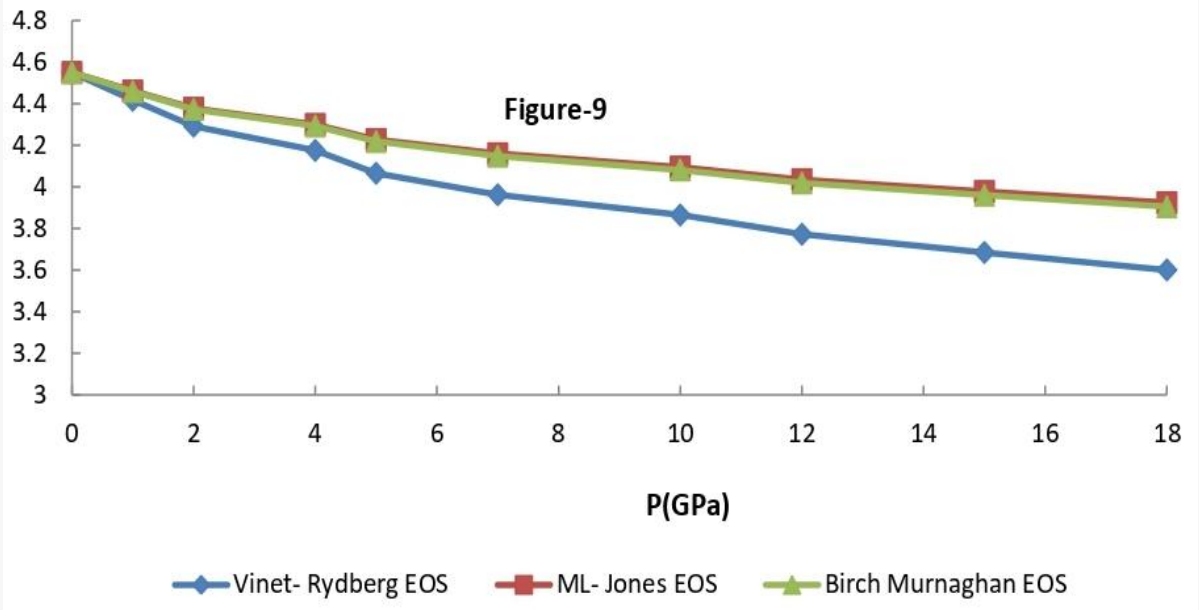


Figure 9 represents the graph between pressure and first pressure derivative of Bulk modulus ($K_T^{'}$) for ZnSe. We notice that $K_T^{'}$ decreases continuously on increasing pressure. The theoretical calculation has been made using three different EOSs (Vinet Rydberg EOS, Modified Lenard Jones EOS and Birch- Murnaghan EOS). This theoretical graph completely satisfies the fact that on increasing pressure volume $K_T^{'}$ decreases [1, 2].

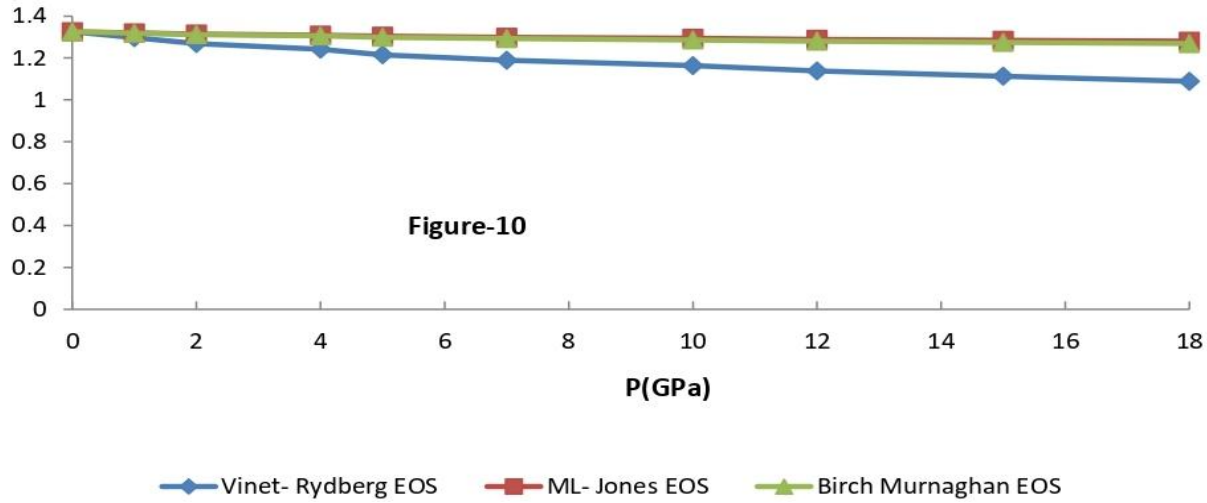


Figure 10 represents the graph between pressure and Gruneisen parameter for ZnSe. Here, we notice that Gruneisen parameter declines with pressure. The theoretical calculation has been made using three different EOSs (Vinet Rydberg EOS, Modified Lenard Jones EOS and Birch- Murnaghan EOS). This theoretical graph completely satisfies the fact that on increasing pressure volume Gruneisen parameter decreases [1,2].

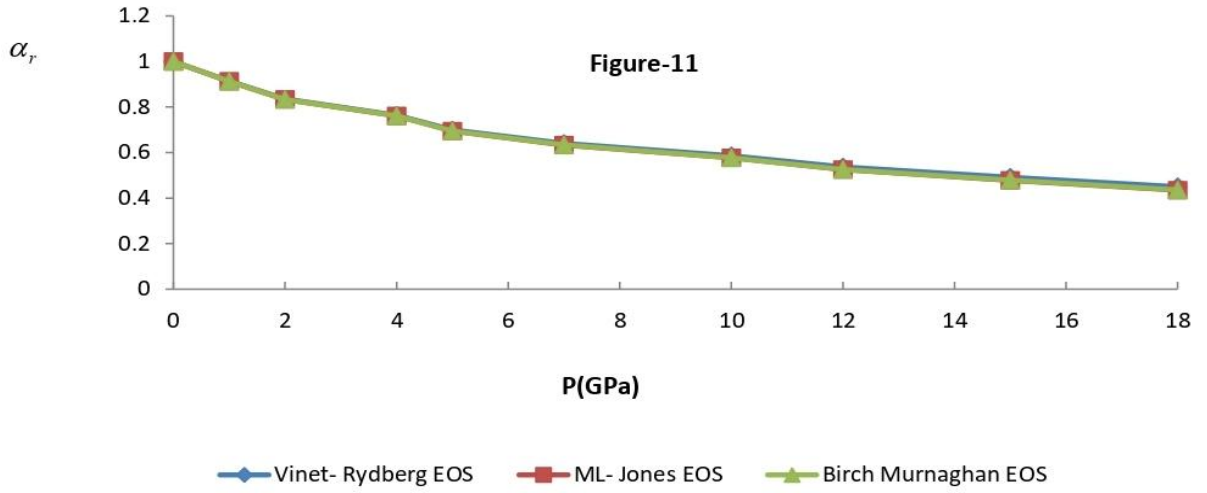


Figure 11 represents the graph between pressure and Relative isothermal expansion coefficient (α_r) for ZnSe. . Here, we notice that α_r declines with pressure. We also notice that α_r decreases by 57% of its initial value when pressure increased by 18GPa. The theoretical calculation has been made using three different EOSs (Vinet Rydberg EOS, Modified Lenard Jones EOS and Birch- Murnaghan EOS). From the above graph we can see that the three equations give exactly same results even at high pressure.

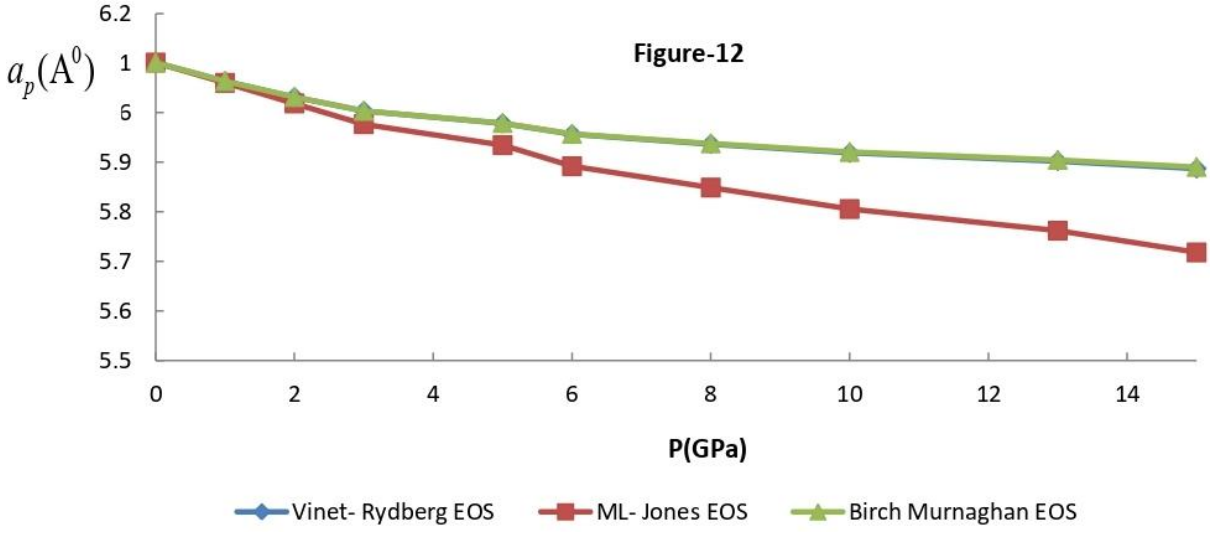


Figure 12 represents the graph between pressure and lattice parameter for ZnSe. The theoretical calculation has been made using three different EOSs (Vinet Rydberg EOS, Modified Lenard Jones EOS and Birch- Murnaghan EOS). From this graph we can also notice that lattice parameter decreases at high pressure

Theoretical Prediction of Structural Properties of ZnTe:

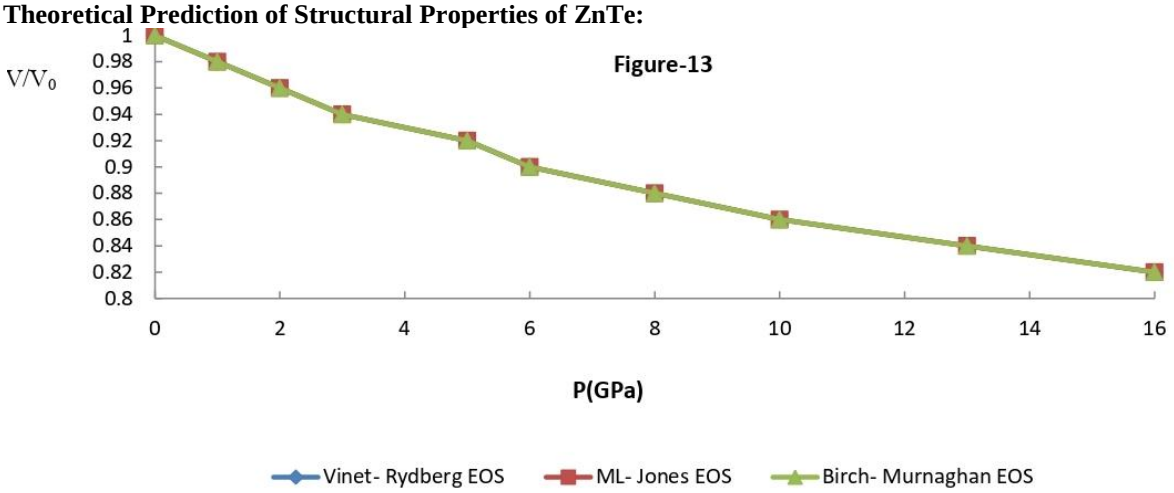


Figure 13 represents the graph between pressure and volume compression ratio for ZnTe. Almost 16GPa pressure is needed so that its volume decrease by 18% from initial value. The theoretical calculation has been made using three different EOSs (Vinet Rydberg EOS, Modified Lenard Jones EOS and Birch- Murnaghan EOS). This theoretical graph completely satisfies the fact that on increasing pressure volume decreases [1, 2].

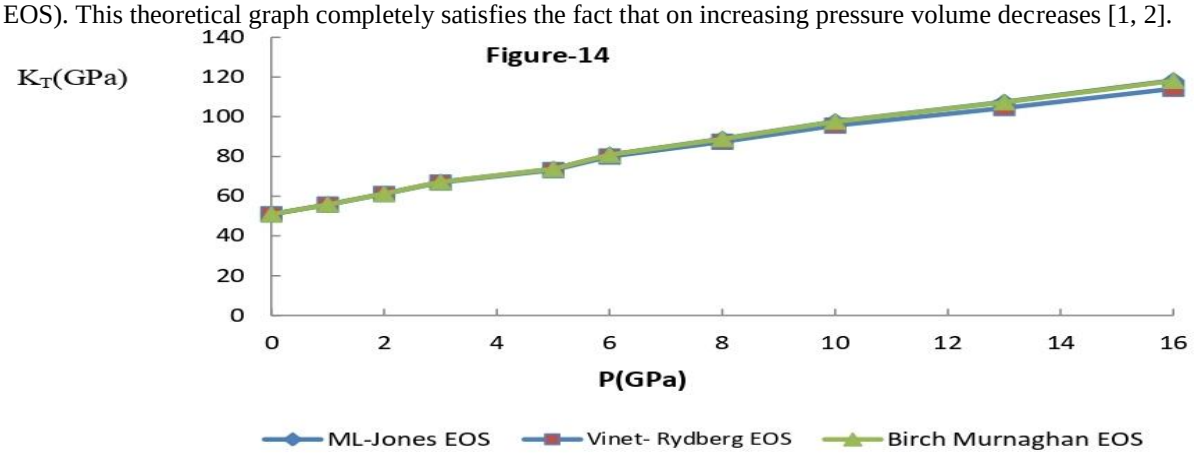


Figure 14 represents the graph between pressure and Bulk modulus (K_T) for ZnTe. Here, we notice that K_T increased by almost 125% from its initial value when pressure increases to 16GPa. The theoretical calculation has been made using three different EOSs (Vinet Rydberg EOS, Modified Lenard Jones EOS and Birch-Murnaghan EOS). This theoretical graph completely satisfies the fact that on increasing pressure volume Bulk modulus increases [1, 2].

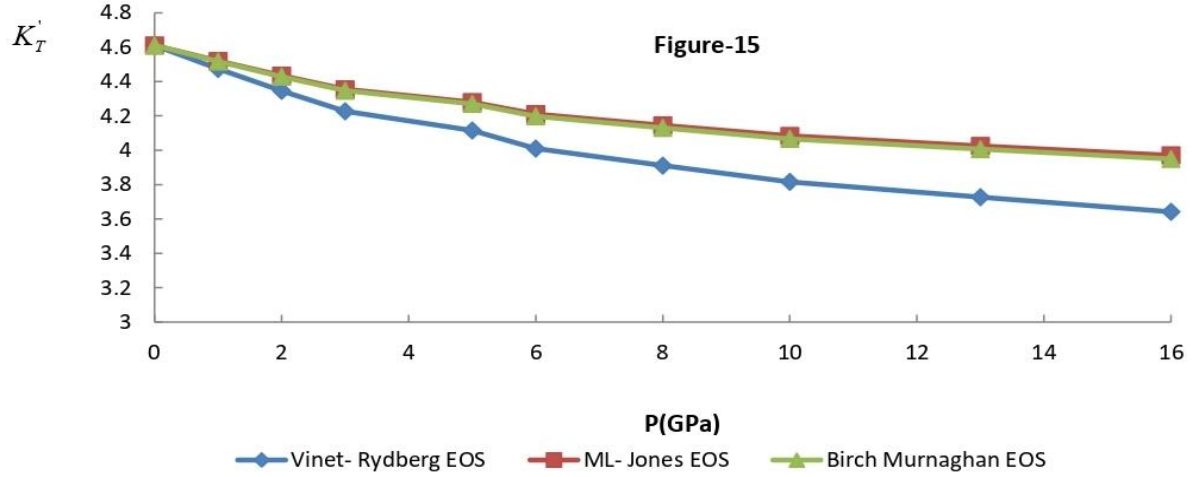


Figure 15 represents the graph between pressure and first pressure derivative of Bulk modulus ($K_T^{'}$) for ZnTe.

We notice that $K_T^{'}$ decreases continuously on increasing pressure. The theoretical calculation has been made using three different EOSs (Vinet Rydberg EOS, Modified Lenard Jones EOS and Birch- Murnaghan EOS). This theoretical graph completely satisfies the fact that on increasing pressure volume $K_T^{'}$ decreases [1,2].

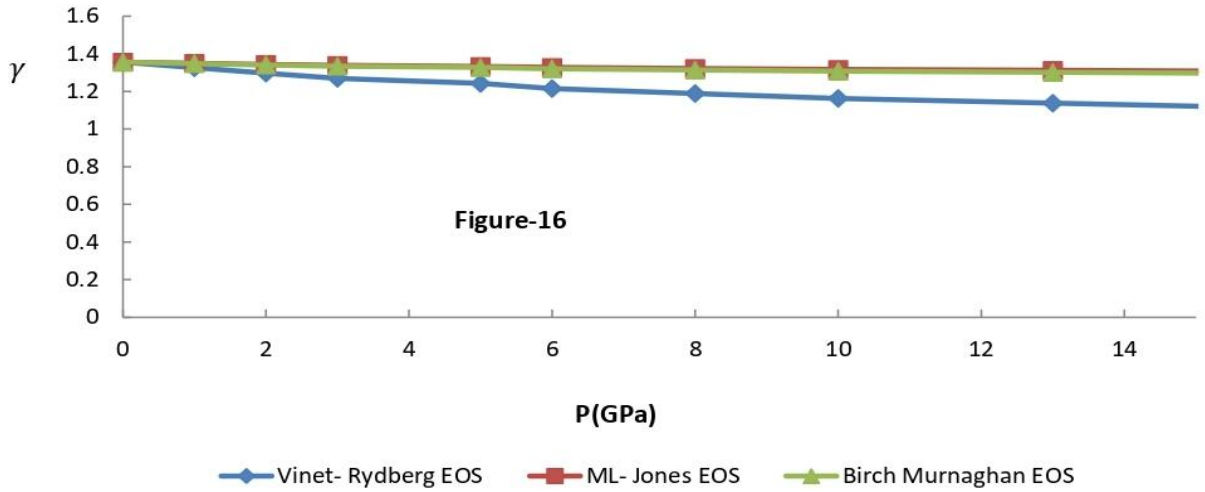


Figure 16 represents the graph between pressure and Gruneisen parameter for ZnTe. Here, we notice that Gruneisen parameter declines with pressure. The theoretical calculation has been made using three different EOSs (Vinet Rydberg EOS, Modified Lenard Jones EOS and Birch- Murnaghan EOS). This theoretical graph completely satisfies the fact that on increasing pressure volume Gruneisen parameter decreases [1,2].

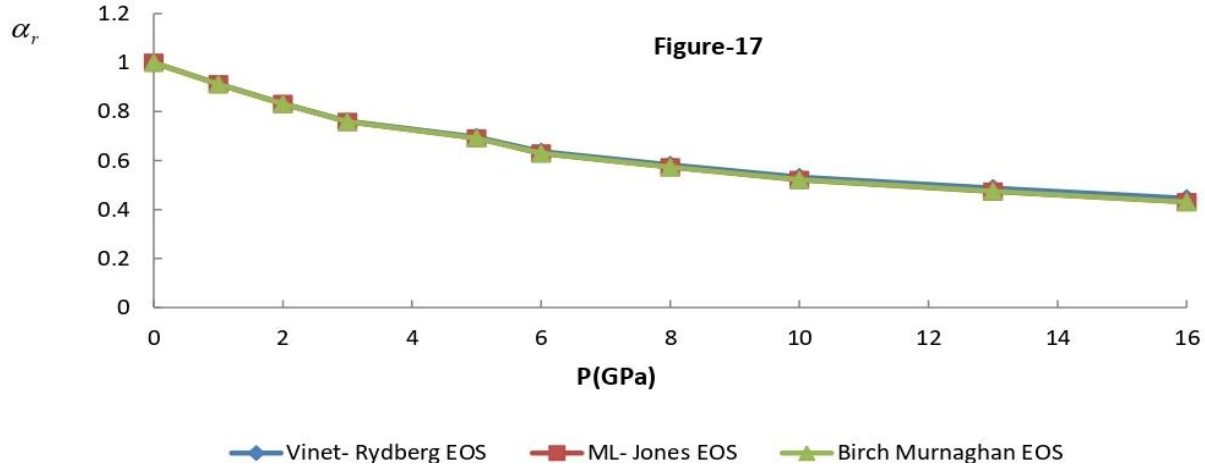
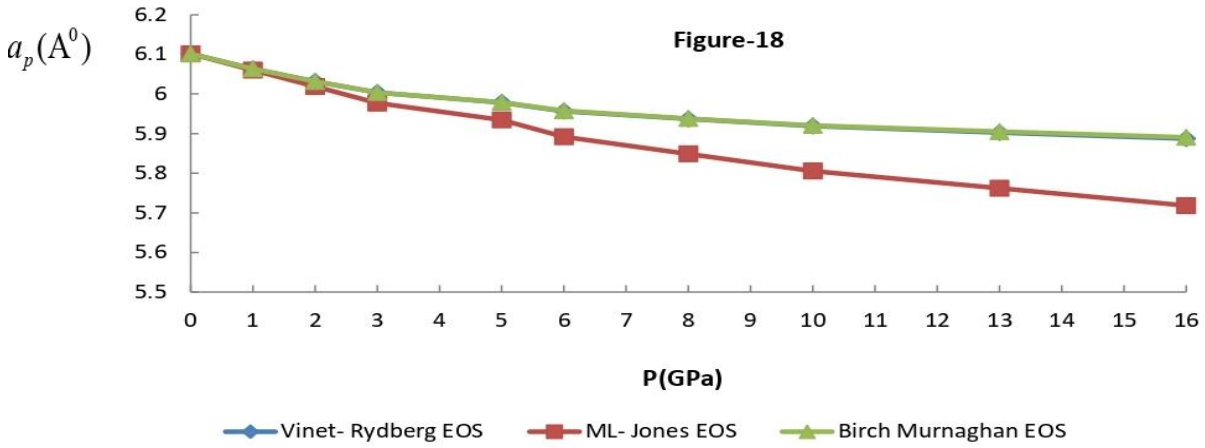


Figure 17 represents the graph between pressure and Relative isothermal expansion coefficient (α_r) for ZnTe. We also notice that α_r decreases by 57% of its initial value when pressure increased by 16GPa.The theoretical calculation has been made using three different EOSs (Vinet Rydberg EOS, Modified Lenard Jones EOS and Birch- Murnaghan EOS). From the above graph we can see that the three equations give exactly same results even at high pressure.



In figure 18, we observe the pressure-lattice parameter relationship for ZnTe. The lattice parameter reduces significantly under high pressure conditions. Theoretical calculations, employing three distinct EOSs (Vinet Rydberg EOS, Modified Lenard Jones EOS, and Birch-Murnaghan EOS), have been utilized to generate this graph.

Conclusion:

In the course of our discussion, several noteworthy conclusions have emerged. To compress the materials by 18% from their original volume, we require pressures of 24GPa for ZnS, 18GPa for ZnSe, and 16GPa for ZnTe, respectively. Among these, ZnS demands the highest pressure, reaching 24GPa. This can be attributed to the high bulk modulus (K0 = 78GPa) of ZnS compared to the other two semiconductors. It is worth noting that the pressure values obtained are consistent, showing no significant deviation. Interestingly, we find that the values for bulk modulus (KT) remain remarkably similar at different pressures for all three materials. This observation leads us to the conclusion that all three equations of state (EOSs) are suitable for calculating the variation of bulk modulus with pressure for these semiconductors. Additionally, we note that to increase KT by approximately 125% from its initial value, we would need pressures of approximately 24GPa for ZnS, 18GPa for ZnSe, and 16GPa for ZnTe. Moreover, the first pressure derivative of bulk modulus continuously decreases as the pressure increases. Furthermore, the Vinet-Rydberg EOS shows slight deviation from the other two EOSs used in our current study. Intriguingly, the Gruneisen parameter diminishes with increasing pressure, and the corresponding graphs appear as almost straight lines. This leads to the conclusion that the ratio of γ/P (where P represents pressure) for the Grüneisen parameter remains constant for ZnS, ZnSe, and ZnTe semiconductors. Furthermore, the relative thermal expansion coefficient decreases with increasing pressure, and the values obtained from all three EOSs for a specific semiconductor are consistent. From this, we deduce that to reduce the value of 57% from its initial value, we would need pressures of 24GPa for ZnS, 18GPa for ZnSe, and 16GPa for ZnTe, respectively. Lastly, we observe that the lattice parameter decreases with pressure in all cases. Moreover, the values obtained from the modified Lenard Jones EOS show slight deviation from the other two EOSs.

References:

1. S Srivastava, A.K Pandey, & C.K Dixit, Theoretical prediction for thermoelastic properties of carbon nanotubes (CNTs) at different pressure or compression using equation of states. J Math Chem. 61, 2098 (2023)
2. S. Srivastava, A K. Pandey, C K Dixit, computational condensed matter 35, e00801 (2023)
3. Kabita, K., Sharma, B. I, Journal of Physics: Conference Series 759, (2016).
4. Yang J, Xue C, Yu S H, Zeng J H and Qian Y T, Angew. Chem. 114, 4891(2002)
5. Peng Q, Dong Y J and Li Y D, Angew. Chem. Int. Edn 42, 3027(2003)
6. Jiuxun Sun, J. Phys. : Condensed Matter 17, (12), L103-L111 , (2005).
7. Vinet P, Ferrante J, Smith J R and Rose J H, J. Phys. C, 92, L467,(1986)
8. A.K Pandey, C.K Dixit S Srivastava, Prachi Singh, Shipra Tripathi, Theoretical prediction of Thermo-Elastic Properties of TiO_2 (Rutile Phase), Natl. Acad. Sci. Lett. (2023)
9. Birch, F, Finite elastic strain of cubic crystals, Phys. Rev. 71, 809, (1947)
10. Borelius G, Solid State Physics (Edited by F. Seitz and D. Turnbull), Academic Press, New York 6, 65. (Cited in : Freund J. and Ingalls R., 1989), (1958)
11. Barton M A and Stacey F D, Phys. earth Planet Interior, 39, 167, (1985)
12. I. O. Radi; , M.A.Abdulsatter; M. Abdul-Lettif , Phys. Stat. Sol. b, 244(4), 1304 (2007).
13. S. K. Jalal, A. M. Al-Sheikh, Raf. J. Sci.,25(.3), 80, (2014)
14. W.A. Harrison, Electronic Structure and the Properties of Solids, Freeman, New York, (1980).
15. Tan J., Li Y., Ji G., Computational materials science 58, 243-247 (2012)
16. Numerical Data and Functional Relationships in Science and Technology, edited by O. Madelung, Landolt-Börnstein, New Series, Group III, Vol. 22, Pt. a (Springer, Berlin, 1987).