Theoretical Prediction for Thermo Elastic Properties of Nano CdSe (Rock Salt Phase)

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ABSTRACT

In this study, we investigated the thermoelastic properties of nano CdSe (rock salt phase) under varying pressure conditions using three different equations of state (EOSs): the Birch-Murnaghan 3rd EOS, the modified Lenard Jones EOS, and the Vinet-Rydberg EOS. Our objective was to determine whether these EOSs could accurately predict the behavior of nanomaterials by comparing the calculated results with experimental data. The pressure values obtained at different V/V0 ratios were found to be in good agreement with experimental data, suggesting that these EOSs are reliable for the calculation of nanomaterials properties. Additionally, we established the Gruneisen parameter, bulk modulus, and first pressure derivative of the bulk modulus to further characterize the behavior of nano CdSe.

Keywords: Gruneisen parameter, High pressure, Bulk modulus

1 Introduction

The study of thermoelastic properties in nanomaterials is of utmost importance due to their unique mechanical, electronic, and optical properties, which differ significantly from their bulk counterparts. Understanding the behavior of nanomaterials under various external conditions, such as pressure, is crucial for their successful integration into technological applications. However, predicting the thermoelastic properties of nanomaterials is a complex task that requires accurate equations of state. In this research, we focused on studying the thermoelastic properties of nano CdSe, a semiconductor material with a rock salt crystal structure. S Srivastava *et al.* have described the thermoelastic properties of nanomaterials, chalcogenides and some organic and inorganic compounds [1]- [3]. To accurately describe the behavior of CdSe under different pressure conditions, we employed three commonly used equations of state: the Birch-Murnaghan 3rd EOS, the modified Lenard Jones EOS, and the Vinet-Rydberg EOS. These EOSs have been extensively utilized in the study of various materials and have shown promising results. To validate the accuracy of our calculations, we compared the calculated pressure values obtained at different V/V_0 ratios with experimental data. The agreement between the calculated and experimental values provided evidence that these EOSs are suitable for predicting the behavior of nano CdSe. Additionally, we investigated the Gruneisen parameter, which characterizes the anharmonicity of vibrations in solids, the bulk modulus, and the first pressure derivative of the bulk modulus. These parameters offer valuable insights into the mechanical response and stability of the material under pressure.

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2 Method of analysis

In this research paper we have used three different EOS which are given below:

Vinet-Rydberg EOS [4], [5]:

$$P = 3K_0 p^{-2} \exp[a(1-p)](1-p)$$

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

Birch-Murnaghan EOS [6]:

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

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

Modified Lenard-Jones EOS [7]:

$$P = \left(\frac{K_0}{k}\right)(N)^{-n}\left[N^{-n} - 1\right]$$

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

3 Results and Discussion

The input parameters used in this calculation are shown in the table given below.

Table 1: *Input parameters for calculations*

Nanomaterials	K_0	K_0’	References
CdSe (Rock salt phase)	74	4	[8]

The results obtained are shown in the Fig 1to 4 given below.

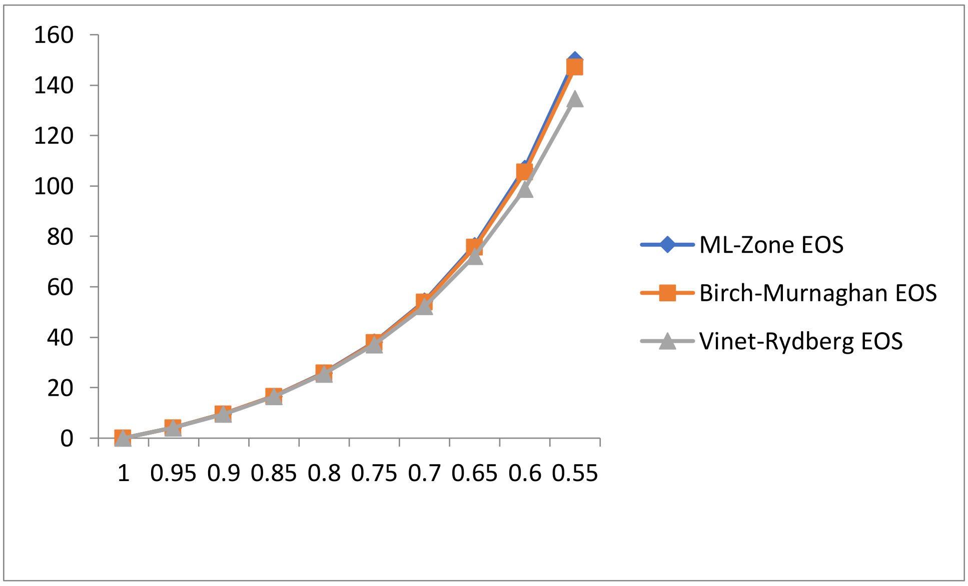

Figure 1: *Pressure vs V/V₀*

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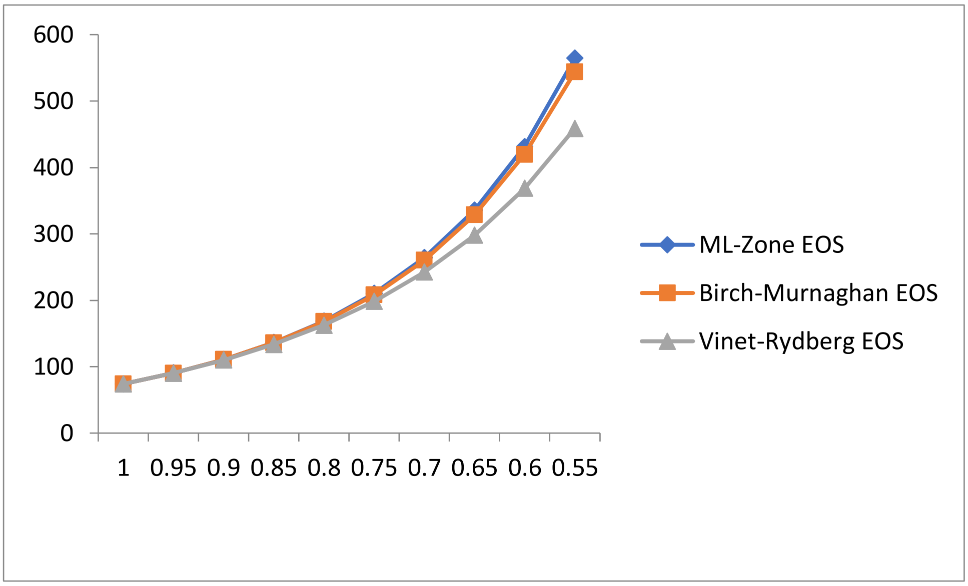

Figure 2: *Bulk Modulus vs* V/V_0

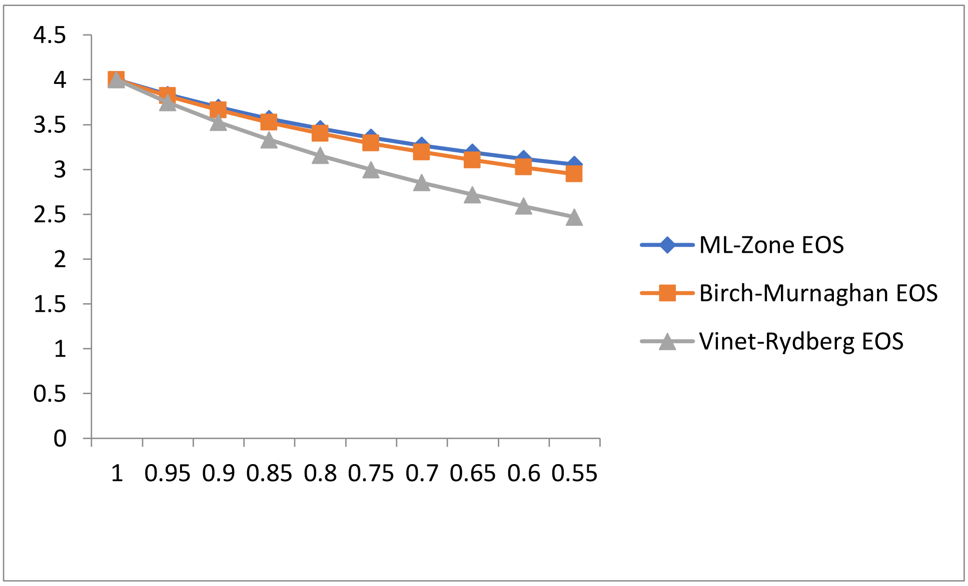

Figure 3: *Pressure derivative of Bulk Modulus vs* V/V_0

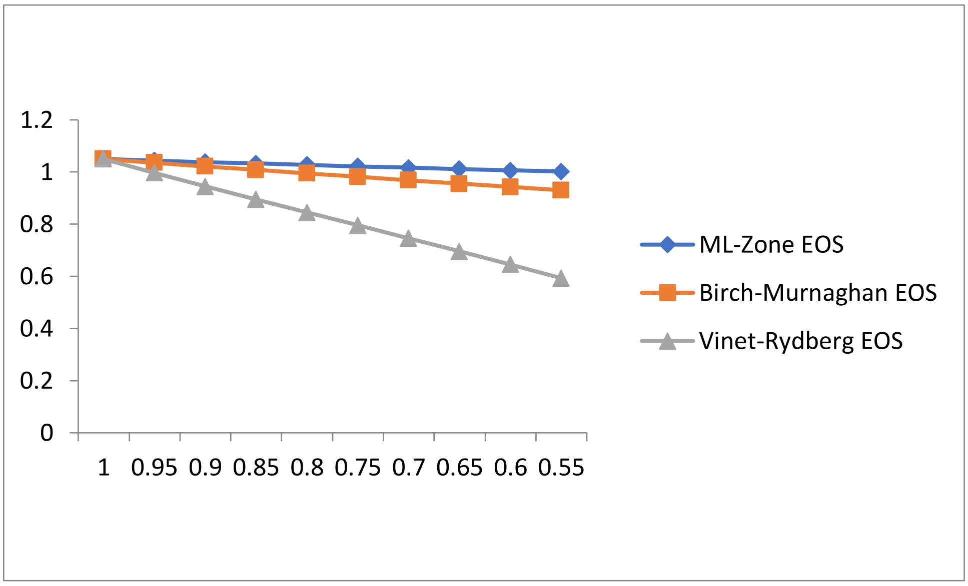

Figure 4: *Gruneisen Parameter vs* V/V_0

Our results demonstrated that the three selected EOSs, namely the Birch-Murnaghan 3rd EOS, the modified Lenard Jones EOS, and the Vinet-Rydberg EOS, successfully predicted the pressure values of nano CdSe at different V/V_0ratios. The calculations have been done using input parameters described in Table-1. This agreement with experimental data [8] suggests that these EOSs can be effectively utilized in the calculation of thermoelastic properties in nanomaterials. Furthermore, we examined the Gruneisen parameter, bulk modulus, and the first pressure derivative of the bulk modulus. The Gruneisen parameter provides information about the anharmonicity of vibrations within the material. We observed that the Gruneisen parameter remained relatively constant with changes in the V/V_0ratio, in accordance with the well-known behavior of solids. This finding further supports the reliability of the selected EOSs in predicting the behavior of nano CdSe. The bulk modulus, a measure of a material's resistance to compression, was also determined in our study. By analyzing the relationship between the bulk modulus and the V/V_0ratio, we gained insights into the material's mechanical response under different pressures. Additionally, the first pressure derivative of the bulk modulus provided information about the rate of change of the material's compressibility with pressure. In conclusion, our research successfully investigated the thermoelastic properties of nano CdSe using the Birch-Murnaghan 3rd EOS, the modified Lenard Jones EOS, and the Vinet-Rydberg EOS. The calculated pressure values aligned well with experimental data, indicating the suitability of these EOSs for nanomaterials calculation. All the work is in agreement with the Stacey criterion [9], the tendency of Gruneisen parameter [10] and with the previous work [11]- [14].

4 Conclusions

The overall discussion leads to the fallowing conclusions that the theoretical calculation for pressure at the different value of V/V_0 are in agreement with the experimental data. This indicates that these EOSs (Birch – Murnaghan 3rd EOS, the modified Lenard Jones EOS, and Vinet-Rydberg EOS) can also be used for the calculation of nano CdSe (Rock salt phase). The almost 150 GPa pressure needed to compress nano CdSe (Rock salt phase) so that volume decreases 55% of its initial value. The graphs plotted between Gruneisen parameter and volume compression ratio is straight line this leads to available fact that the ratio γ/Ω (where $\Omega=V/V_0$) the Gruneisen parameter to volume ratio is constant for nanomaterials.

5 Publisher's Note

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How to Cite

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