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Theoretical Prediction of Thermo Elastic Properties of Semiconductor Nanomaterials under High Compression

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Abstract
Thermoelastic properties of semiconductor nanomaterials are directly connected with the isothermal equation of states (EOS). The EOS of a system establishes a relationship between thermodynamical variables at different pressures. In this paper, we have theoretically predicted the value of bulk modulus, its first pressure derivative and the Grüneisen parameter (γ) for InP, InAs, and InSb under different compression values (V/V0). The analysis of pressure-volume compression relationships revealed linear growth in pressure with compression, indicating nanocrystal contraction. The results of this study contribute valuable insights into nanomaterial mechanics, emphasizing the significance of EOS selection and compression range for accurate predictions in materials science applications.
***Keywords**: Equation of States (EOSs); Semiconductor Nanomaterials; High-pressure; Bulk modulus; Grüneisen parameter (γ)*

I. Introduction

Semiconductor Nanomaterials are getting very high attention in these days as they are considered the heart of next technological revolution of world. The study of thermo elastic properties of semiconductor nanomaterial attracted the attention of both experimental and theoretical researchers as the thermo elastic properties are backbone of both the mechanical and thermodynamic properties of nanomaterial. Thermo elastic properties of nanomaterials are directly connected with the isothermal equation of states (EOS). The EOS of a system establishes a relationship between thermodynamical variables at different pressure, so we shall study the thermo elastic properties of InP (Indium phosphide), InAs (Indium arsenide) and InSb (Indium antimonide) with the help of different EOSs Theoretical researchers have introduced different isothermal equation of state for calculation of pressure, bulk modulus, pressure derivative of bulk modulus, Grüneisen Parameter, etc. at different compressions. The Grüneisen parameter is a dimensionless quantity which is related to the anharmonicity of lattice vibrations.

Where the band gaps of semiconductors materials are InP in (1.42 eV),InAs in (0.43eV), and InSb in (0.23) [1]. It is consist of nature (III-V) has themolecular formula InP, InAs, and InSb belongs to the direct semiconductors material family with main industrial interest [2]. In the current study we have used three different isothermal equation of state for theoretical prediction of Grüneisen parameter for InP, InAs and InSb. The isothermal EOS of a system is very useful for studying the properties of materials at different compression ratio (V/V0) or at different pressures. The behavior of nanomaterials under different compression ratio (V/V0) can give important information about their fundamental micro structural properties [3]. Since at high compression thermo elastic properties of nanomaterials can change, so high compression is also an interesting research field within nanoscale. Further nanomaterials are very sensitive to temperature, pressure and volume changes. As we know that the theoretical efforts are much useful to understand the behavior of nano- materials under compression. In this paper, we have theoretically predicted the value of bulk modulus, its first pressure derivative of bulk modulus and the value of Grüneisen parameter for InP, InAs, and InSb under different compression values (V/V0). We have used three different isothermal EOSs viz. Birch- Murnaghan EOS, Brennan- Stacey EOS and Vinet-Rydberg EOS for theoretical prediction of Grüneisen parameter.

Method of analysis: In this study, we have used three different EOSs.
(1) Birch – Murnaghan (3rd-order) EOS derived using finite strain theory [4].
(2) Brennan- Stacey EOS derived using thermodynamic formulation for Grüneisenparameter [5, 6].
(3) Vinet-Rydberg EOS based on the universal relationship between binding energy and interatomic separation for solids [7, 8].

These EOSs are given below

$$\mathbf{P} = \frac{3}{2}\mathbf{K0}(\mathbf{x}^{-7} - \mathbf{x}^{-5})\left[\mathbf{1} + \frac{3}{2}(\mathbf{K'0} - \mathbf{4})(\mathbf{x}^{-2} - \mathbf{4})\right] (\mathbf{1})$$

$$\boldsymbol{P} = \frac{\mathbf{3}\boldsymbol{K0x^{-4}}}{(\mathbf{3}\boldsymbol{K'}\mathbf{0} - \mathbf{5})}\left[\mathbf{exp}\left\{\frac{(\mathbf{3K'0} - \mathbf{5})(\mathbf{1} - \mathbf{x}^{3})}{\mathbf{3}}\right\} - \mathbf{1}\right] (\mathbf{2})$$

$$\boldsymbol{P} = \mathbf{3}\boldsymbol{K0x^{-2}}(\mathbf{1} - \boldsymbol{x})\boldsymbol{exp}[\boldsymbol{\eta}(\mathbf{1} - \boldsymbol{x})] \qquad (\mathbf{3})$$

Where $\boldsymbol{X} = \left(\frac{V}{V0}\right)^{1/3}$ and $\boldsymbol{\eta} = \frac{3}{2}(\boldsymbol{K'}\mathbf{0} - \mathbf{1})$.

Equation (1) is Birch – Murnaghan (3rd-order) EOS, equation (2) is Brennan-Stacey EOS and equation (3) isVinet-Rydberg EOS. Where V is the volume at pressure P and V0 is the volume at zero pressure, K0 is isothermal bulk modulus at zero pressure and K0 first pressure derivative of isothermal bulk modulus at zero pressure.The two parameters are correlated according to equation of state theory [9].Isothermal bulk modulus can be calculated by above equations using formula: $\mathbf{Kt} = -\mathbf{V}\left(\frac{\partial P}{\partial V}\right)\boldsymbol{t}$[8]

From equations (1)-(3) and following expressions can be obtained:

$$\boldsymbol{Kt} = \frac{\boldsymbol{K0}}{\mathbf{2}}[\mathbf{7}\boldsymbol{x}^{-7} - \mathbf{5}\boldsymbol{x}^{-5}] + \frac{\mathbf{3}}{\mathbf{8}\boldsymbol{K0}}(\boldsymbol{K'}\mathbf{0} - \mathbf{4})(\mathbf{9}\boldsymbol{x}^{-9} - \mathbf{14}\boldsymbol{x}^{-7} + \mathbf{5}\boldsymbol{x}^{-5})(\mathbf{4})$$

$$\boldsymbol{Kt} = \boldsymbol{K0x^{-1}}\mathbf{exp}[(\boldsymbol{K'}\mathbf{0} - \frac{\mathbf{5}}{\mathbf{3}})(\mathbf{1} - \boldsymbol{x}^{3}) + \frac{\mathbf{4}}{\mathbf{3}}\boldsymbol{p} \qquad (\mathbf{5})$$

$$\boldsymbol{Kt} = \boldsymbol{K0x^{-2}}[\mathbf{1} + (\boldsymbol{\eta x} + \mathbf{1})(\mathbf{1} - \boldsymbol{x})]\mathbf{exp}[\boldsymbol{\eta}(\mathbf{1} - \boldsymbol{x})] \qquad (\mathbf{6})$$

Now expression for, K'T (The first order pressure derivative of bulk modulus) can be obtains by using formula: $\boldsymbol{K't} = \left(\frac{\partial Kt}{\partial P}\right)\boldsymbol{t}$

$$\boldsymbol{K't} = \frac{K0}{8Kt}\left[(\boldsymbol{K'}\mathbf{0} - \mathbf{4})(\mathbf{81}\boldsymbol{x}^{-9} - \mathbf{98}\boldsymbol{x}^{-7} + \mathbf{25}\boldsymbol{x}^{-5}) + \frac{4}{3}(\mathbf{49}\boldsymbol{x}^{-7} - \mathbf{25}\boldsymbol{x}^{-5})\right](\mathbf{7})$$

$$\boldsymbol{K't} = \left(\mathbf{1} - \frac{\mathbf{4}\boldsymbol{P}}{\mathbf{3}\boldsymbol{Kt}}\right)\left[\left(\boldsymbol{K'}\mathbf{0} - \frac{\mathbf{5}}{\mathbf{3}}\right)\boldsymbol{x}^{3} + \frac{\mathbf{5}}{\mathbf{3}}\right] + \frac{\mathbf{16}\boldsymbol{P}}{\mathbf{9}\boldsymbol{Kt}} \qquad (\mathbf{8})$$

$$\boldsymbol{K't} = \frac{\mathbf{1}}{\mathbf{3}}\left[\frac{\boldsymbol{x}(\mathbf{1} - \boldsymbol{\eta}) + \mathbf{2}\boldsymbol{\eta x^{2}}}{\mathbf{1} + (\mathbf{1} + \boldsymbol{\eta x})(\mathbf{1} - \boldsymbol{x})} + \boldsymbol{\eta x} + \mathbf{2}\right] \qquad (\mathbf{9})$$

The value of Grüneisen parameter (γ) can be calculated by using theformula given by Borton and Stacey [10]

$$\boldsymbol{\gamma} = \frac{\left(\frac{1}{2}\right)\boldsymbol{K't} - \frac{1}{6} - \frac{f}{3}\left[\mathbf{1} - \frac{1}{3}\left(\frac{P}{Kt}\right)\right]}{\mathbf{1} - \left(\frac{4}{3}\right)\left(\frac{P}{Kt}\right)} \qquad (\mathbf{10})$$

Where, F=2.35

II. Results and discussion

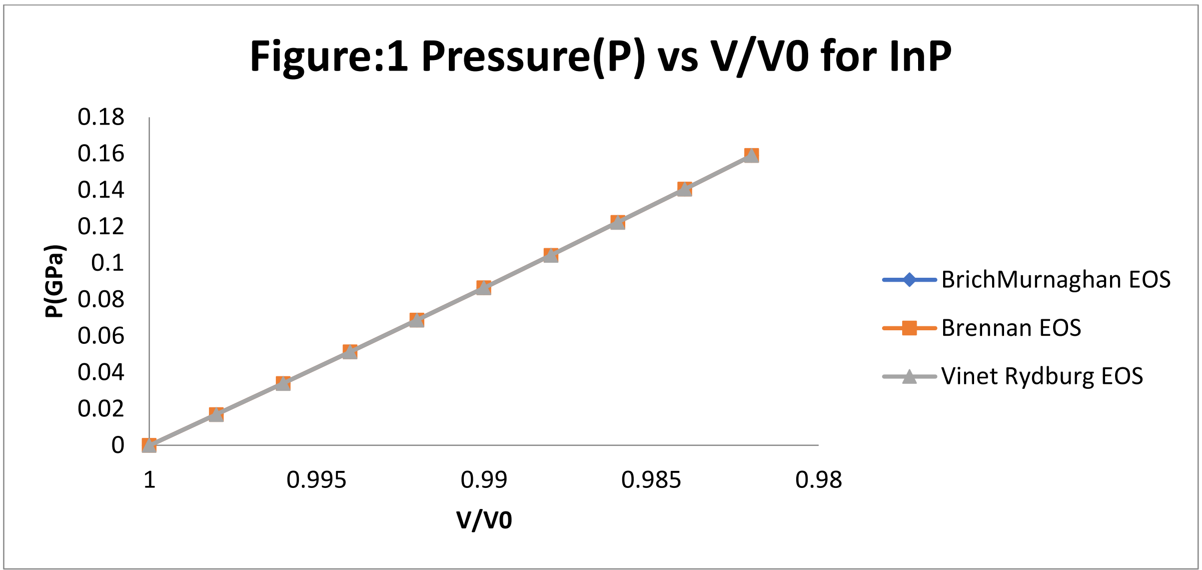
In this work we have describe three different isothermal equation of states viz.Birch-Murnaghan equation of state, Brennan-Staceyequation of state and Vinet-Rydberg equation of state for calculatingpressure, isothermal bulk modulus, first pressure derivative ofisothermal bulk modulus and Grüneisen parameter at different compressions the value of Pressure (P) are calculated by usingequation (1-3). The input value of K0and K'0 are shown in Table 1.Further using the value are P in equation (4-6) We find value of KTfurther substituting the values are P and KT calculated by usingequation (1-6) in equation (7-9) we find the values of K'T furthersubstituting the values of P, KTand K'T obtain from equation (1-9) inequation (10) we obtain the value of Gruneisen parameter. The graphsare plotted between the calculated values of P at differentcompressions by using Birch-Murnaghan EOS, Brennan-Stacey EOSand Vinet-Rydberg EOS is shown in Figures 1-3. Further the graphplotted between V/V0 and KT are shown in Figures 4-6, the graphplotted between V/V0and K'T are shown in Figures 7-9 and also thegraph plotted between V/V0and Gruneisen parameter (γ) are shown in

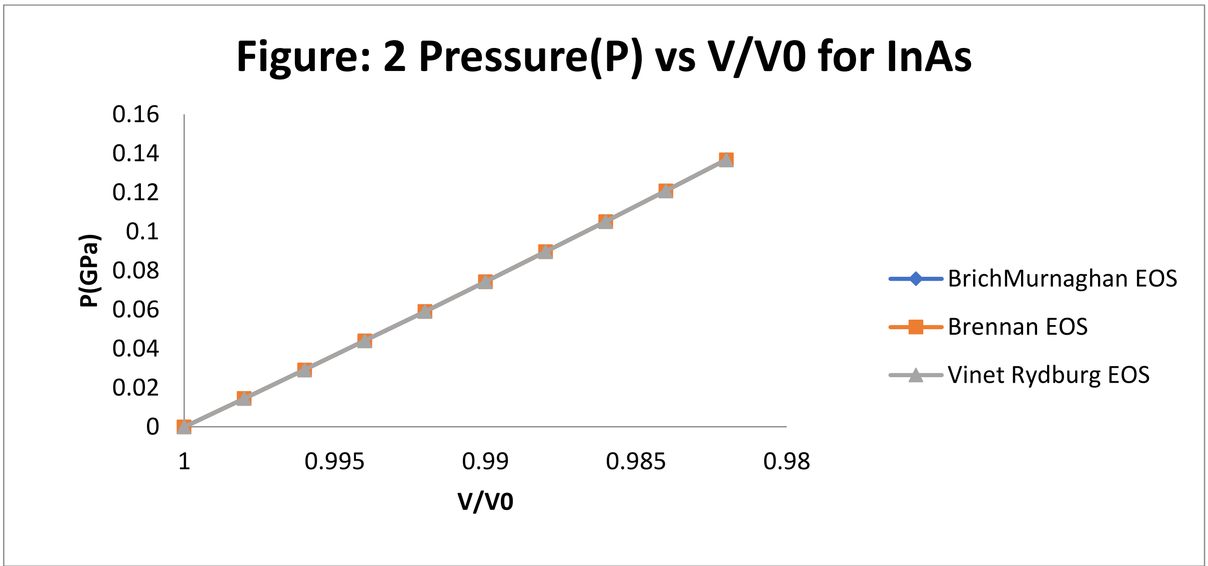
Figures10-12. Equation (1), (4) and (7) represent the BirchMurnaghan 3rd order EOS's. Equation(2), (5) and (8) represent the Brennan-Stacy EOS's and Equation (3), (6) and (9) represent the Vinet-Rydberg EOS's and equation (10)represent the Gruneisen parameter respectively [15-18].

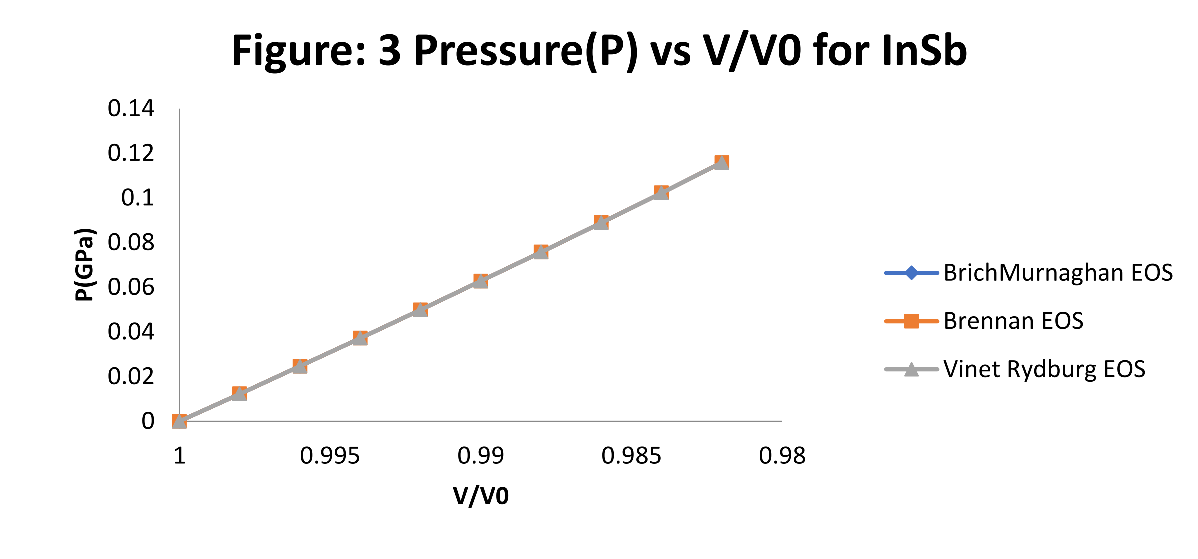
Table-1: values of input data for K0 and K'0 is shown

Nanomaterial	K0 (GPa)	K'0	Reference
InP	8.41	4.43	[27]
InAs	7.23	4.56	[27]
InSb	6.08	5.18	[27]

A graph plotted between P vs V/V0 for InP, InAs, and, InSb are shown inFigures 1-3.

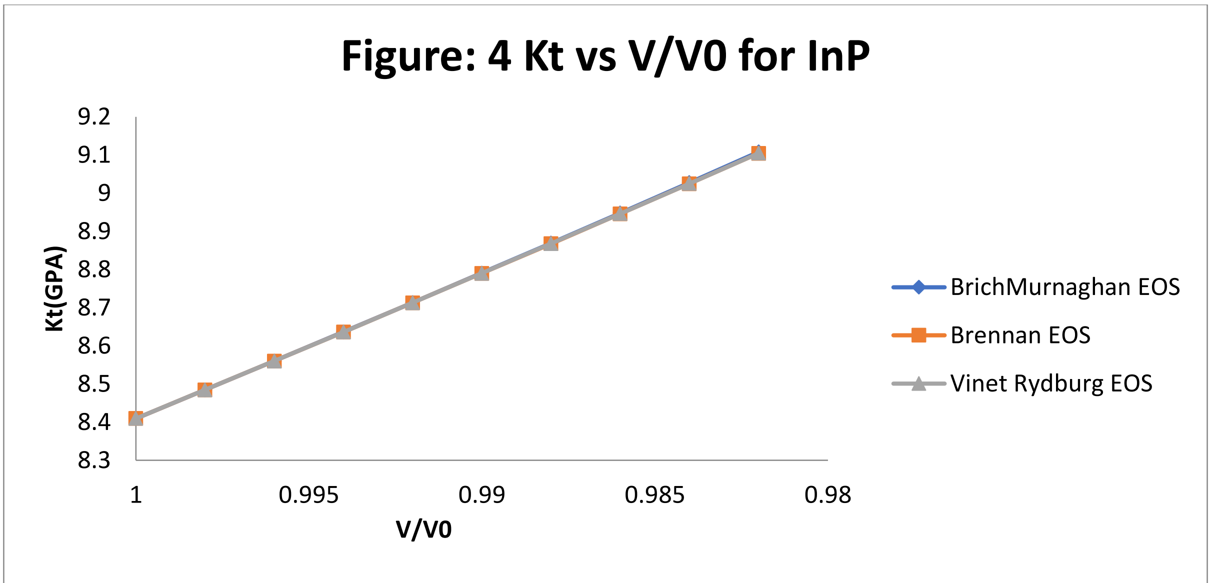


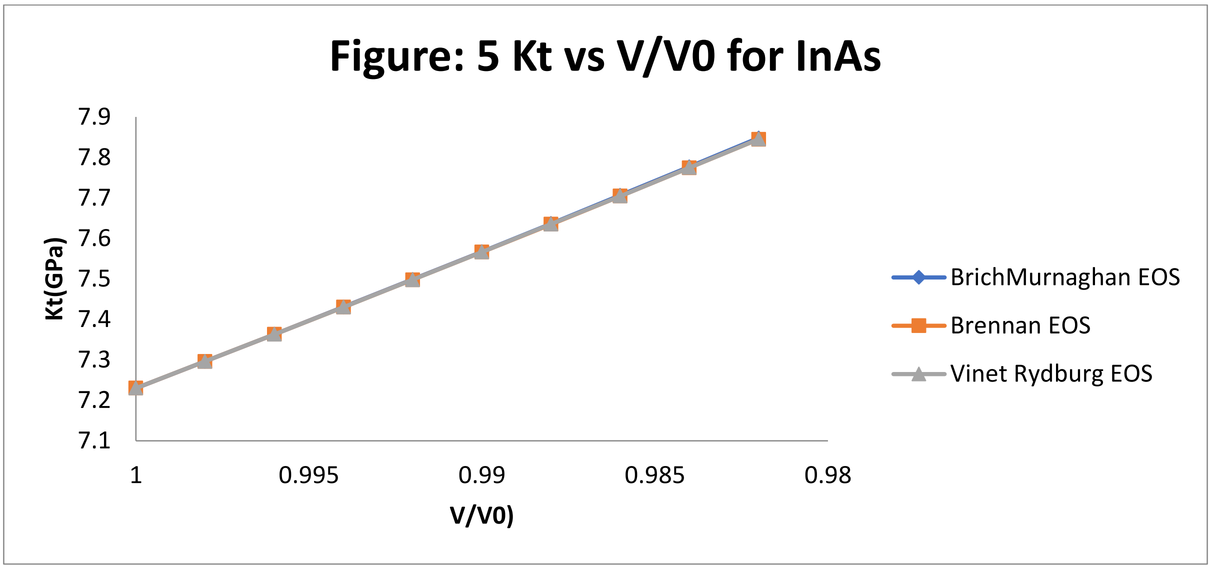


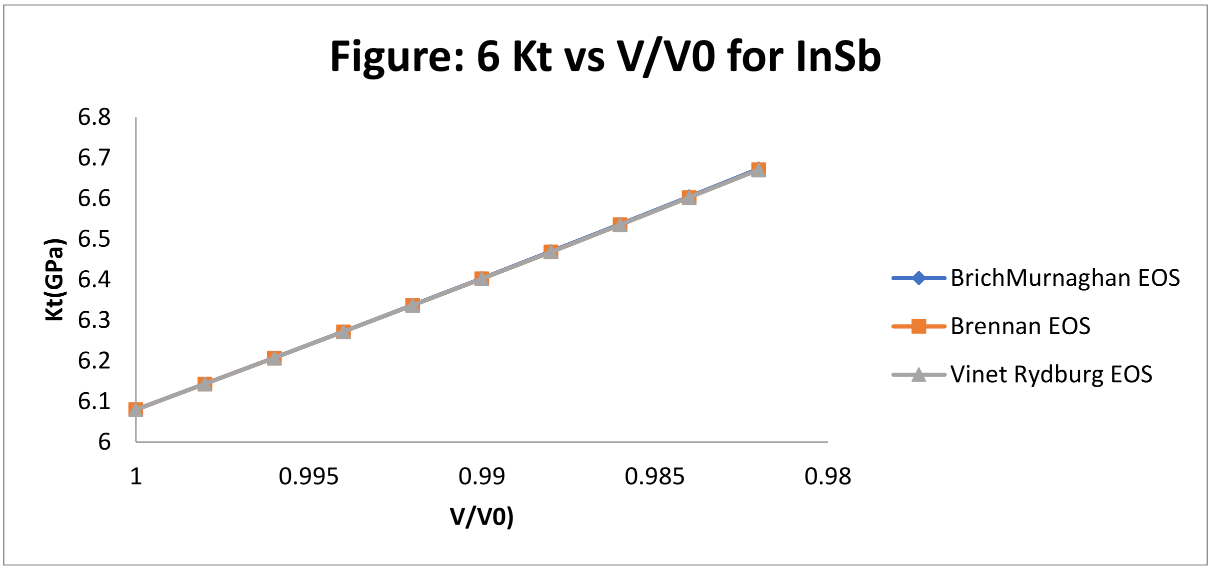


From above the value of Pressure at different compressions is shown in Figures 1-3. From Figures (1),(2)&(3), it is clear that with increasing the compressionsthe value of Pressure increases linearly which verifies the observe fact that with increasing pressures the nanocrystals gets contracted or compressions ratio increases. Further from critical study of the graph it is observe that for InPthe three EOSs corresponds well upto volume compressions range (V/V0)=1,at pressure (P)=0.16GPa, then after the Birch-Murnaghan EOS, Brennan-Stacey EOS and Vinet-Rydberg EOS corresponds well with each other. Whereas for InAs, all the three EOSs corresponds well upto volume compressions range (V/V0)=1, at pressure (P)=0.14GPa, then after the Birch-Murnaghan EOS,Brennan-Stacey EOS and Vinet-Rydberg EOS corresponds well with each other. Similarly for InSball the three EOSs corresponds well upto volume compressions range (V/V0)=1,at pressure (P)=.12GPa, then after the Birch-Murnaghan EOS ,Brennan-Stacey EOS and Vinet-Rydberg EOS corresponds well with each other over entire compressions range [19-21].

Further the graph for isothermal bulk modulus vs V/V0 for InP, InAs, and, InSb are shown in Figures 4-6.







From above The value of Bulk modulus at different compression are shown in figures (4), (5) and (6),it is clear that with increasing the compression the value of bulk modulus increases linearly which verifies the observe fact thatwith increasing bulk modulus the nanocrystals gets contracted or compression ratio increases.Further from critical study of the graph it is observe that for InP all the three EOSs corresponds well upto volume compressions range (V/V0)=1,at isothermal bulk modulus (Kt)=9.1GPa, then after the Birch-Murnaghan EOS ,Brennan-Stacey EOS and Vinet-Rydberg EOS corresponds well with each other. Whereas for InAs and InSb all the three EOSs corresponds well upto volume compressions range (V/V0)=1, at isothermal bulk modulus(Kt)=7.9GPa and compressions range (V/V0) =1 at isothermalbulkmodulus6.7GPa, then after the Birch-Murnaghan EOS ,Brennan-Stacey EOS and Vinet-Rydberg EOS corresponds well with each other [22-25].

Further the graph for first pressure derivative of isothermal bulk modulus vs V/V0 for InP, InAs, and, InSb are shown in Figures 7-9.

Figure: 7 First Pressure Derivative of Kt vs V/V0 for InP

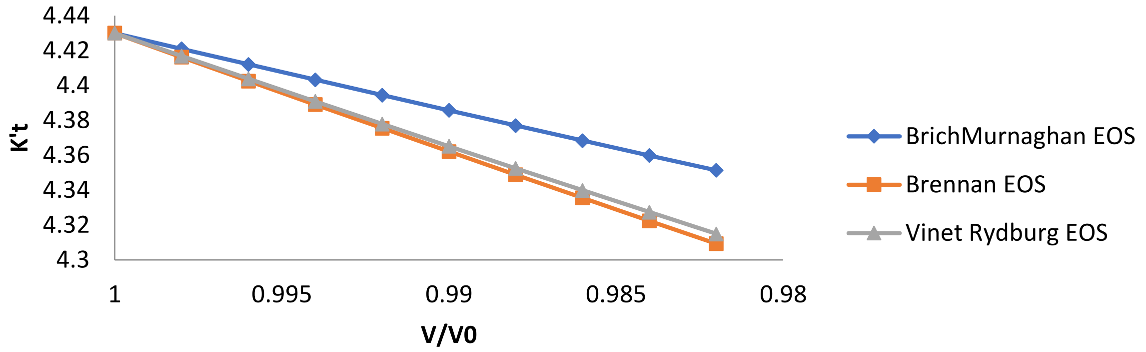
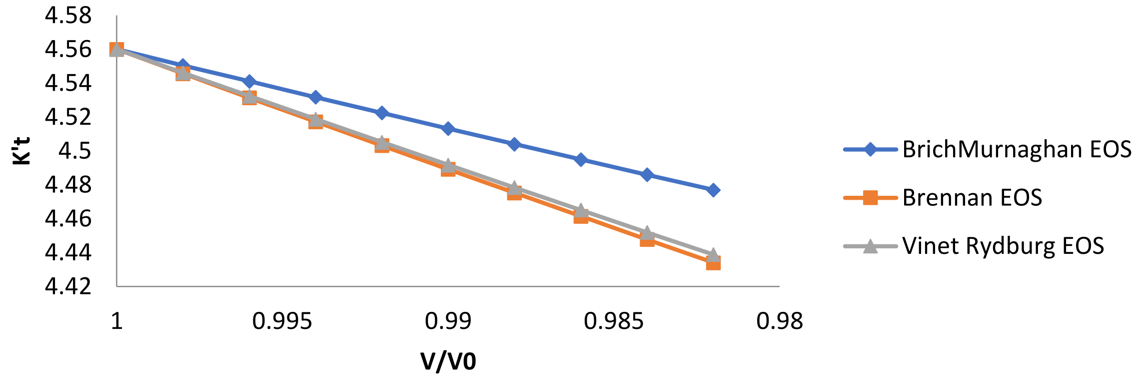
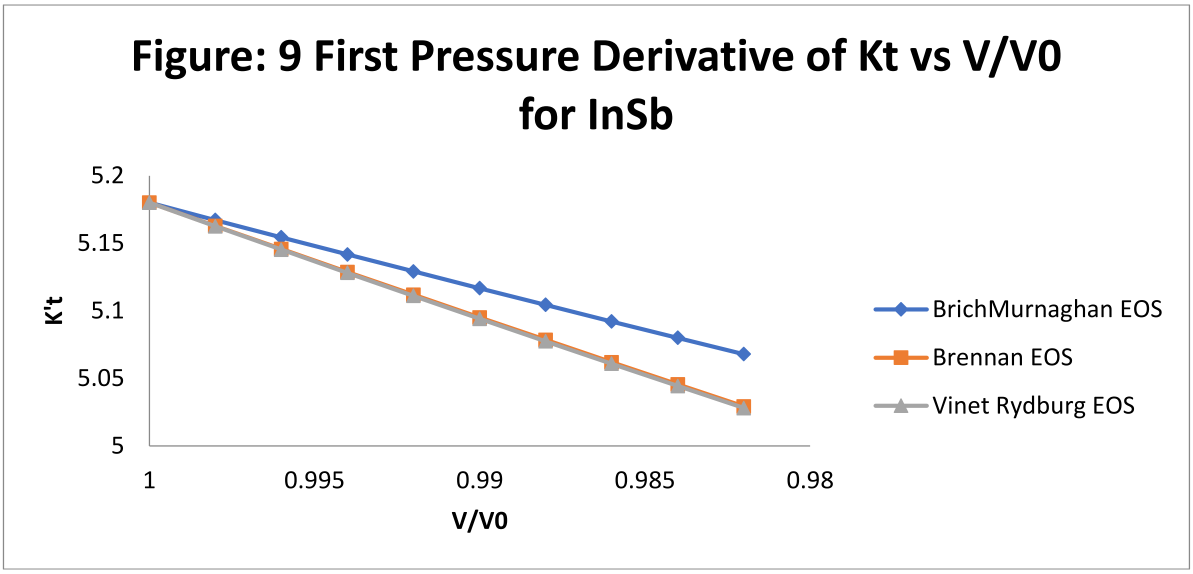


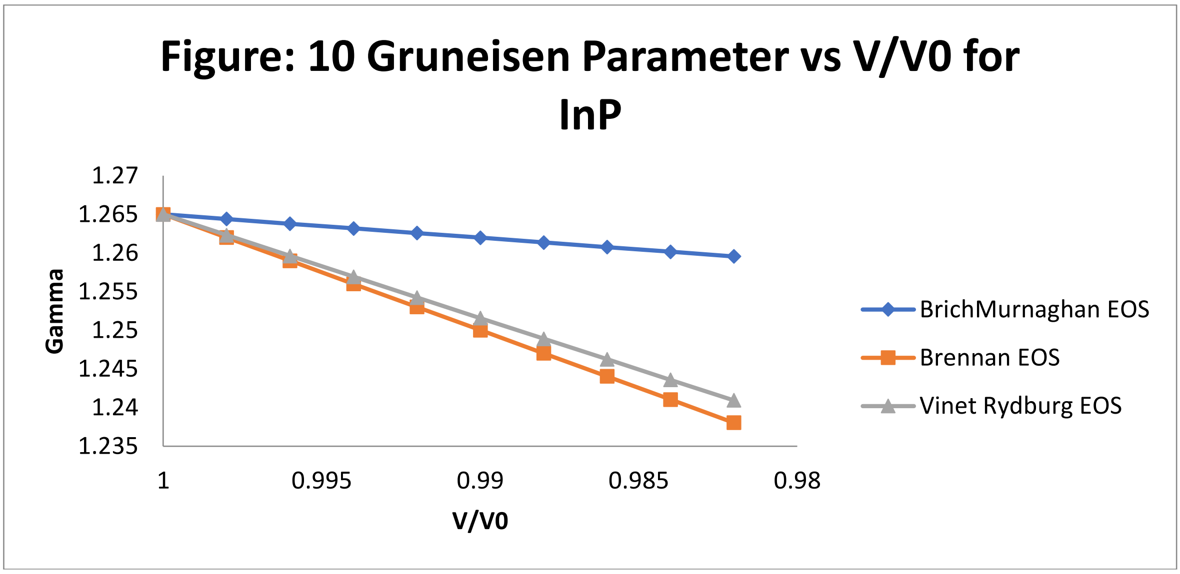
Figure: 8 First Pressure Derivative of Kt vs V/V0 for InAs

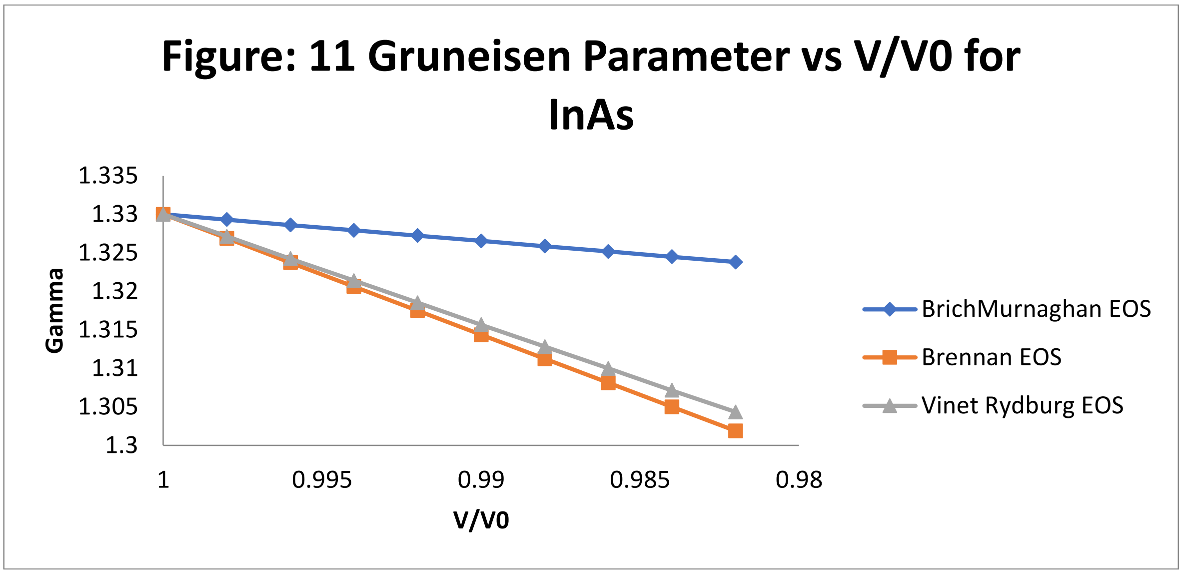


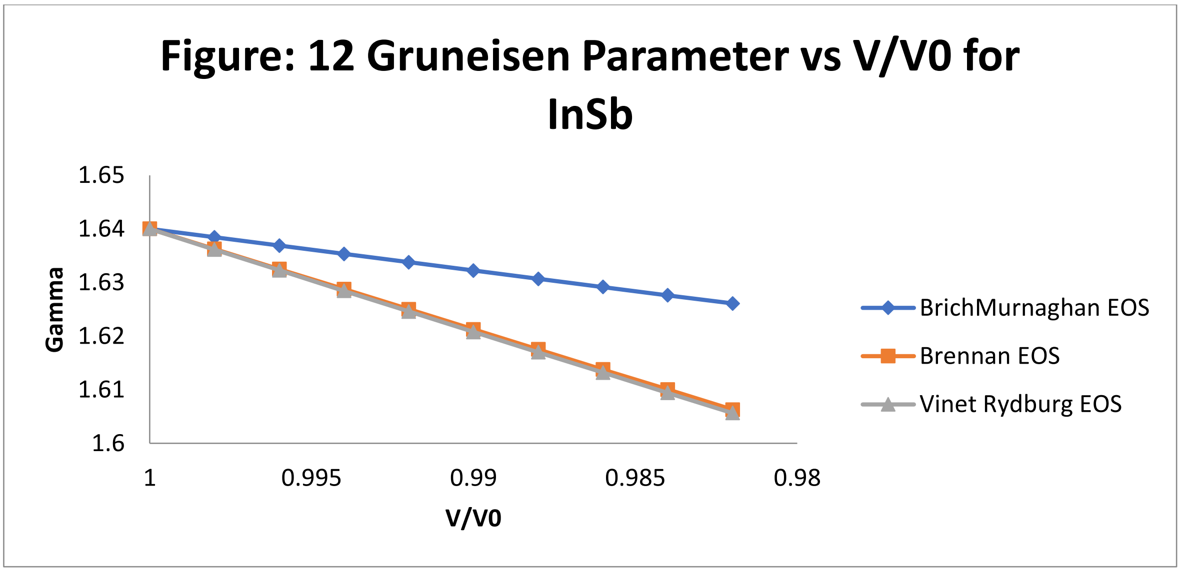


From Figures 7-9 it is clear that on decreasing first pressurederivative of isothermal bulk modulus, the value of compressionincreases for all the three nanomaterials InP, InAs and InSb. Further for InPthe Brennen-Stacey EOS and Vinet-Rydberg EOS corresponds well with each other but the Birch-Murnaghan EOS starts deviating below compression range V/V0=0.997at first pressure derivative of isothermal bulk modulus 4.35GPa with othertwo EOSs. Whereas for InAs and InSb are both the Brennen-Stacey EOS and Vinet-Rydberg EOS corresponds well with each other but the Birch Murnaghan EOS starts deviating below compression range (V/V0) =0.997 at firstpressurederivative of isothermal bulk modulus 4.48 GPA and compression range (V/V0)=0.997 at first pressure derivative of isothermal bulk modulus 5.03 GPawith each other entire compression range .

Further the graph for Gruneisen parameter (γ) vs V/V0 for InP, InAs and InSb are shown in Figures 10-12.







From Figures 10-12 it is clear that on decreasing Gruneisen parameter (γ),the value of compression increases for all the three nanomaterials InP, InAs and InSb. Further for InSb the Brennen-Stacey EOS and Vinet-Rydberg EOS corresponds well with each other but the Birch Murnaghan EOS starts deviating below compression range (V/V0)=.998 at Gruneisen parameter (γ)1.635with other two EOSs. Whereas for InP and InSball the three EOSs(Brennan-StaceyEOS and Vinet-Rydberg EOS and Birch Murnaghan EOS) does not Corresponds with each other entirecompression range[26].

III. Conclusion

To conclude, this research investigated three distinct isothermal equations of state (EOSs) – Birch-Murnaghan, Brennan-Stacey, and Vinet-Rydberg – to evaluate pressure, isothermal bulk modulus (KT), first pressure derivative of isothermal bulk modulus (K'T), and the Grüneisen parameter (γ) for InP, InAs, and InSb nanomaterials across varying compressions. The analysis of pressure-volume compression relationships revealed linear growth in pressure with compression, indicating nanocrystal contraction. Agreement among EOSs was observed within specific compression ranges, affirming their validity. Investigation of isothermal bulk modulus indicated proportional growth with compression. Examination of first pressure derivative of bulk modulus and the Gruneisen parameter demonstrated consistent trends: as K'T and γ decreased, compression increased. Notably, EOS correspondence varied for different materials. These findings contribute valuable insights into nanomaterial mechanics, emphasizing the significance of EOS selection and compression range for accurate predictions in materials science applications.

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