Journal of Information Systems Engineering and Management
2025, 10(59s)
e-ISSN: 2468-4376
https://www.jisem-journal.com/

Research Article

Prediction of Thermodynamic Parameter at High Pressure

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ARTICLE INFO

Received: 29 Dec 2024

Revised: 12 Feb 2025

Accepted: 27 Feb 2025

ABSTRACT

In present work, we have theoretically studied some thermoelastic properties of TiO2 and nano-TiO2 under high pressure, such as pressure, isothermal bulk modulus, and relative isothermal expansion coefficient of materials, by using four different Equation of States (EOSs): viz. (I) Murnaghan EOS, (II) Vinet-Rydberg EOS, (III) Born-Mayer EOS and (IV) M-L Jones EOS. The result showed that the pressures increase as compression increases, which is in excellent agreement with experimental value. The bulk modulus also increases as pressure increases, and the value of relative isothermal expansion coefficient increases as pressure decreases.

Keywords: High Pressure, Equation of states, Isothermal bulk modulus, Relative isothermal expansion coefficient

INTRODUCTION

Many experiments have been conducted to study and interpret the behaviour of nanomaterials. It is not surprising that the theoretical study of high-pressure investigations into nanomaterials has developed alongside the growth of nanoscience. This progress has been driven by the dual objectives of achieving a better understanding of nanomaterial properties and providing alternative approaches for the synthesis and manipulation of nanostructures [1-10]. The application of varying pressures to a wide range of solid-state materials plays a crucial role in advancing the study of nanomaterials. High-temperature and high-pressure conditions offer unique opportunities to explore new materials in unprecedented ways. Applying pressure to bulk materials alters interatomic interactions within nano-objects, creating an invaluable tool to investigate physical-chemical interactions at the nanoscale and their connection to material properties of interest [11-28]. The physical properties of materials are heavily influenced by their structure and interatomic distances. High pressure can modify these distances, enabling researchers to study the relationships between a material's structure and its properties in detail. When high pressure is applied to nanomaterials, it induces several notable effects, including: (a) Transformation of nano-component elements, (b) Modification of interactions between the nano-object and the pressure-transmitting medium, and (c) Alteration of interactions between nano-objects [13-28].

Theoretical studies have extensively explored the fundamental physical and chemical properties of various TiO_2 nanomaterials, often considering bulk materials as references. Titanium dioxide (TiO_2), a wide bandgap semiconductor (3.2 eV), belonging to the transition metal oxides family and holding significant industrial interest. Due to its superior physical and chemical properties, TiO_2 nanomaterials have been widely applied in areas such as photocatalysis and dye-sensitized solar cells (DSCs), driving significant research in this field. TiO_2 have numerous applications such as sunscreens to advanced technologies and they play a crucial role in environmental and biomedical fields, including pollutant degradation, water purification, biosensing, and drug delivery. The diverse and impactful nature of these applications has driven significant advancements in the fabrication, characterization, and fundamental understanding of TiO_2 nanomaterials over the past decades. [29-35]

In this present work, we calculated the thermoelastic properties viz. Pressure, isothermal bulk modulus, and relative isothermal expansion coefficient of TiO_2 and nano- TiO_2, by using four different Equation of States (EOSs): viz. (I) Murnaghan EOS, (II) Vinet-Rydberg EOS, (III) Born-Mayer EOS and (IV) M-L Jones EOS at high pressure [36-39].

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METHOD OF ANALYSIS-

We have investigated some thermoelastic properties of TiO_2 and nano- TiO_2 under high pressure. Here, we have used four different isothermal EOSs. Which are given below [16, 36, 40, 41, 42]:

I. Murnaghan EOS – The Murnaghan equation of state was developed by Francis D. Murnaghan in year 1944 [41].

$$P_M = \frac{B_0}{B_0'}\left[\left(\frac{V}{V_0}\right)^{-B_0'} - 1\right] \quad (1)$$

Where P_M is the lower subscript refer to Murnaghan EOS, P is the pressure in GPa. B_0 is isothermal bulk modulus at ambient condition, it is also in GPa. B_0' is first pressure derivative of is isothermal bulk modulus at ambient condition. V is volume under high pressure and V_0 is initial volume at ambient conditions, both are in nanometre (nm).

II. Vinet-Rydberg EOS -

$$P_{(V-R)} = 3B_0x^{-2/3}(1 - x^{1/3})exp[\eta(1 - x^{1/3})] \quad (2)$$

Where $P_{(V-R)}$ is the lower subscript refer to Vinet-Rydberg EOS, P is the pressure in GPa.

Here, $x = \left(\frac{V}{V_0}\right)$ and $\eta = \frac{3}{2}(B_0' - 1)$

III. Born - Mayer EOS -

$$P_{(B-M)} = \frac{3B_0}{\eta-2}\left[\left(\frac{V}{V_0}\right)^{\frac{-2}{3}} exp\left\{\eta\left[1 - \left(\frac{V}{V_0}\right)^{\frac{1}{3}}\right]\right\} - \left(\frac{V}{V_0}\right)^{\frac{-2}{3}}\right] \quad (3)$$

Where $P_{(B-M)}$ is the lower subscript refer to Born - Mayer EOS, P is the pressure in GPa.

Here, $\eta = \frac{3(B_0'-1)}{2} + \left[\frac{9(B_0'-1)^2}{4} - 6B_0' + 12\right]^{1/2}$

IV. Modified Lenard Jones EOS -

$$P_{(M-L\,J)} = \left(\frac{B_0}{n}\right)\left(\frac{V}{V_0}\right)^{-n}\left[\left(\frac{V}{V_0}\right)^{-n} - 1\right] \quad (4)$$

Where $P_{(M-L\,J)}$ is the lower subscript refer to Modified Lenard Jones EOS, P is the pressure in GPa.

Here $n = \frac{B_0'}{3}$

Computation of isothermal bulk modulus (B_T) using different EOSs:

The expression for isothermal bulk modulus (B_T) under high pressure (P) for different isothermal EOSs has been computed on the basis of below mentioned equation [1, 36]

$$B_T = -V\left(\frac{\partial P}{\partial V}\right)_T \quad (5)$$

From above equations (1,2,3 and 4) we can obtain the expression for isothermal bulk modulus (B_T) under high pressure (P) is shown below,

(I). Variation of isothermal bulk modulus $B_{T(M)}$ using Murnaghan EOS (From eq. (1)):

$$B_{T(M)} = -V\left(\frac{\partial P_{(M)}}{\partial V}\right)_T \quad (6)$$

While

$$\left(\frac{\partial P_{(M)}}{\partial V}\right)_T = B_0\left[\left(\frac{V}{V_0}\right)^{-B_0'}\right] \quad (7)$$

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The above eq. 7 can be written as follows

$$B_{T(M)} = B_0\left[\left(\frac{V}{V_0}\right)^{-B_0'}\right] \tag{8}$$

(II). Variation of isothermal bulk modulus $B_{T(V-R)}$ using Vinet-Rydberg EOS (From eq. (2)):

$$B_{T(V-R)} = -V\left(\frac{\partial P_{(V-R)}}{\partial V}\right)_T \tag{9}$$

While

$$\left(\frac{\partial P_{(V-R)}}{\partial V}\right)_T = B_0 x^{-2/3}[1+\{\eta x^{1/3}+1\}(1-x^{1/3})]exp[\eta(1-x^{1/3})] \tag{10}$$

The above eq.10 can be written as follows

$$B_{T\,(V-R)} = B_0 x^{-2/3}[\{1+(\eta x^{1/3}+1)(1-x^{1/3})\}exp\{\eta(1-x^{1/3})\}] \tag{11}$$

(III). Variation of isothermal bulk modulus $B_{T(B-M)}$ using Born-Mayer EOS (From eq. (3)):

$$B_{T(B-M)} = -V\left(\frac{\partial P_{(B-M)}}{\partial V}\right)_T \tag{12}$$

while

$$\left(\frac{\partial P_{(B-M)}}{\partial V}\right)_T = \frac{3B_0}{\eta-2}\left[\frac{\eta}{3}\left(\frac{V}{V_0}\right)^{\frac{-1}{3}} exp\left\{\eta\left[1-\left(\frac{V}{V_0}\right)^{\frac{1}{3}}\right]\right\}+\frac{2}{3}\left(\frac{V}{V_0}\right)^{\frac{-2}{3}} exp\left\{\eta\left[1-\left(\frac{V}{V_0}\right)^{\frac{1}{3}}\right]\right\}-\frac{4}{3}\left(\frac{V}{V_0}\right)^{\frac{-4}{3}}\right] \tag{13}$$

The above eq.13 can be written as follows

$$B_{T(B-M)} = \frac{3B_0}{\eta-2}\left[\frac{\eta}{3}\left(\frac{V}{V_0}\right)^{\frac{-1}{3}} exp\left\{\eta\left[1-\left(\frac{V}{V_0}\right)^{\frac{1}{3}}\right]\right\}+\frac{2}{3}\left(\frac{V}{V_0}\right)^{\frac{-2}{3}} exp\left\{\eta\left[1-\left(\frac{V}{V_0}\right)^{\frac{1}{3}}\right]\right\}-\frac{4}{3}\left(\frac{V}{V_0}\right)^{\frac{-4}{3}}\right] \tag{14}$$

(IV). Variation of isothermal bulk modulus $B_{T(M-L\,J)}$ using Modified Lenard Jones EOS (From eq. (4)):

$$B_{T(M-L\,J)} = -V\left(\frac{\partial P_{(M-L\,J)}}{\partial V}\right)_T \tag{15}$$

while

$$\left(\frac{\partial P_{(M-L\,J)}}{\partial V}\right)_T = B_0\left(\frac{V}{V_0}\right)^{-n}\left[2\left(\frac{V}{V_0}\right)^{-n}-1\right] \tag{16}$$

The above eq. 15 can be written as follows

$$B_{T\,(M-L\,J)} = B_0\left(\frac{V}{V_0}\right)^{-n}\left[2\left(\frac{V}{V_0}\right)^{-n}-1\right] \tag{17}$$

Computation of Relative isothermal expansion coefficient (a_r) –

The change in temperature with the something change of volume describes the coefficient of thermal expansion. Specifically, the measures the ratio between the relative change in volume when a temperature changes. relative isothermal expansion coefficient is [36, 37]

$$a_r = \frac{a}{a_0} \tag{18}$$

While

$$\frac{a}{a_0} = \frac{B_0}{B_T} \tag{19}$$

and above eq. 16 can be written as follows

$$a_r = \frac{B_0}{B_T} \tag{20}$$

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(I). Variation of Relative isothermal expansion coefficient (a_r) at high pressure using Murnaghan EOS -

Substituting eq.8 into eq. 18 and

$$a_{r\,(M)} = \frac{B_0}{B_0\left[\left(\frac{V}{V_0}\right)^{-B_0'}\right]} \tag{21}$$

The above eq. 19 can be written as follows

$$a_{r\,(M)} = \left[\left(\frac{V}{V_0}\right)^{B_0'}\right] \tag{22}$$

(II). Variation of Relative isothermal expansion coefficient (a_r) at high pressure using Vinet-Rydberg EOS -

Substituting eq. 8 into eq. 11 and

$$a_{r\,(V-R)} = \frac{B_0}{B_0 x^{-2/3}[1+\{\eta x^{1/3}+1\}(1-x^{1/3})]exp[\eta(1-x^{1/3})]} \tag{23}$$

The above eq. 21 can be written as follows

$$a_{r\,(V-R)} = x^{2/3}\left[\{1+(\eta x^{1/3}+1)(1-x^{1/3})\}exp\{\eta(1-x^{1/3})\}\right]^{-1} \tag{24}$$

(III). Variation of Relative isothermal expansion coefficient (a_r) at high pressure using Born-Mayer EOS

Substituting eq. 8 into eq. 14 and

$$a_{r\,(B-M)} = \frac{B_0}{\frac{3B_0}{\eta-2}\left[\frac{\eta}{3}\left(\frac{V}{V_0}\right)^{\frac{-1}{3}} exp\left\{\eta\left[1-\left(\frac{V}{V_0}\right)^{\frac{1}{3}}\right]\right\}+\frac{2}{3}\left(\frac{V}{V_0}\right)^{\frac{-2}{3}} exp\left\{\eta\left[1-\left(\frac{V}{V_0}\right)^{\frac{1}{3}}\right]\right\}-\frac{4}{3}\left(\frac{V}{V_0}\right)^{\frac{-4}{3}}\right]} \tag{25}$$

The above eq. 25 can be written as follows

$$a_{r\,(B-M)} = \frac{\eta-2}{3}\left[\frac{\eta}{3}\left(\frac{V}{V_0}\right)^{\frac{-1}{3}} exp\left\{\eta\left[1-\left(\frac{V}{V_0}\right)^{\frac{1}{3}}\right]\right\}+\frac{2}{3}\left(\frac{V}{V_0}\right)^{\frac{-2}{3}} exp\left\{\eta\left[1-\left(\frac{V}{V_0}\right)^{\frac{1}{3}}\right]\right\}-\frac{4}{3}\left(\frac{V}{V_0}\right)^{\frac{-4}{3}}\right]^{-1} \tag{26}$$

(IV). Variation of Relative isothermal expansion coefficient (a_r) at high pressure using Modified Lenard Jones EOS

Substituting eq. 8 into eq. 17 and

$$a_{r\,(M-L\,J)} = \frac{B_0}{B_0\left(\frac{V}{V_0}\right)^{-n}\left[2\left(\frac{V}{V_0}\right)^{-n}-1\right]} \tag{27}$$

The above eq. 28 can be written as follows

$$a_{r\,(M-L\,J)} = \left(\frac{V}{V_0}\right)^{n}\left[2\left(\frac{V}{V_0}\right)^{-n}-1\right]^{-1} \tag{28}$$

RESULT & DISCUSSION

- In this present work we have discussed the four different equation of states viz. (I) Murnaghan EOS, (II) Vinet-Rydberg EOS (III) Born-Mayer EOS and (IV) M-L Jones EOS for calculating the thermoelastic properties of materials viz. pressure at various compressions, isothermal bulk modulus and relative isothermal expansion coefficient under high pressure for TiO_2 and nano-TiO_2. The pressure is calculated by using equations (1,2,3 and 4) and isothermal bulk modulus calculated by using equation (8,11,14 and 17) and the relative isothermal expansion coefficient calculated by using equation (22,24,26 and 27). Isothermal bulk modulus (B_0) and first derivative of isothermal bulk modulus (B_0') at zero pressure are two parameters present in all EOSs. It has been usual practice to adjust or to fit the parameters in order to achieve the agreement with the experimental values and its numeric value shown in table 1. Further finding the value of P we are using the value of B_0 and B_0' in equation (1,2,3,4) at different compressions. We find the value of B_T Further substituting the values of P and B_T calculated by using equations (8,11,14 and 17). Further, we find the value of the relative isothermal expansion coefficient under high pressure calculated by using

Journal of Information Systems Engineering and Management
2025, 10(59s)
e-ISSN: 2468-4376
https://www.jisem-journal.com/

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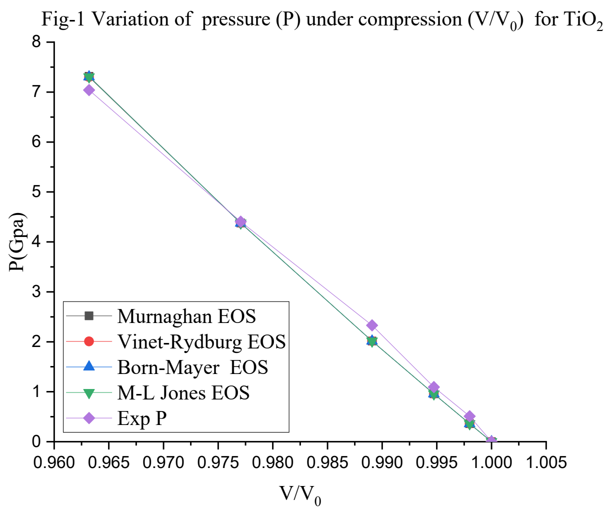
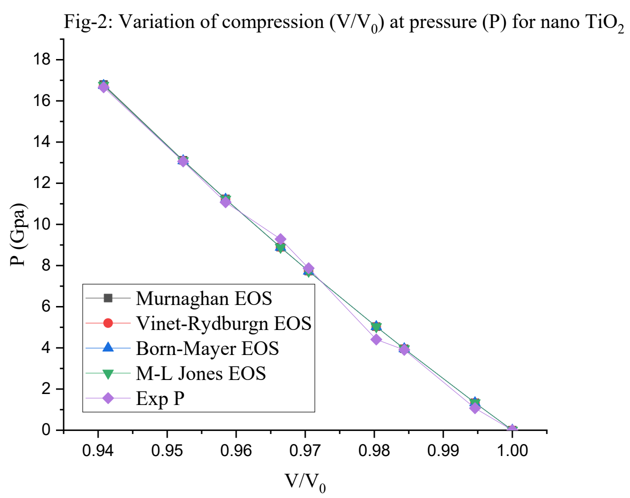
equations (22, 24, 26 and 28). The graphs plotted between the calculated value of P and experimental value of P at different compressions by using Murnaghan EOS, Vinet-Rydberg EOS, Born-Mayer EOS and M-L Jones EOS are shown in figures (1 and 2). Further, the graphs plotted between the calculated value of B_T under high pressure and the graph of B_T are shown in figures (3 and 4). Furthermore, the calculated value of relative isothermal expansion coefficient (a_r) under high pressure and the graph of a_r are shown in figures (5 and 6). The equations (1,8 and 22) represent the Murnaghan EOS. The equations (2, 11 and 24) represent the Vinet-Rydberg EOS, the equations (3,14 and 26) represent the Born-Mayer EOS, the equations (4, 17 and 28) represent the M-L Jones EOS and the equations (18,19 and 20) represent relative isothermal expansion coefficient respectively.

Table. 1 Input parameters of isothermal bulk modulus and first pressure derivative is given below.

S. No.	Nanomaterial	B_0	B_0'	Reference
1	TiO_2	179	4.5	[32]
2	Nano-TiO_2	243	4	[32]

A graph plotted between Pressure with compression for TiO_2 and Nano-TiO_2





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2025, 10(59s)
e-ISSN: 2468-4376
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From figures (1 and 2) it is clear that increasing the pressure leads to an increase in the compression value for TiO_2 and nano-TiO_2. Furthermore, for TiO_2 all EOSs show good agreement with experimental pressure values, but all EOSs slightly deviated in all the compression ranges, and somewhere in all the compression range, all the EOSs fully matched with experimental pressure to computed pressure. For nano-TiO_2 initially shows slightly different experimental pressure values up to a volume compression range $(V/V_0) = 0.96$ at 10 GPa; subsequently, all the EOSs show excellent agreement with experimental values.

A graph plotted between isothermal bulk modulus under high pressure for TiO_2 and Nano-TiO_2

Fig-3: Variation of Bulk modulus (B_T) at high pressure (P) for TiO_2

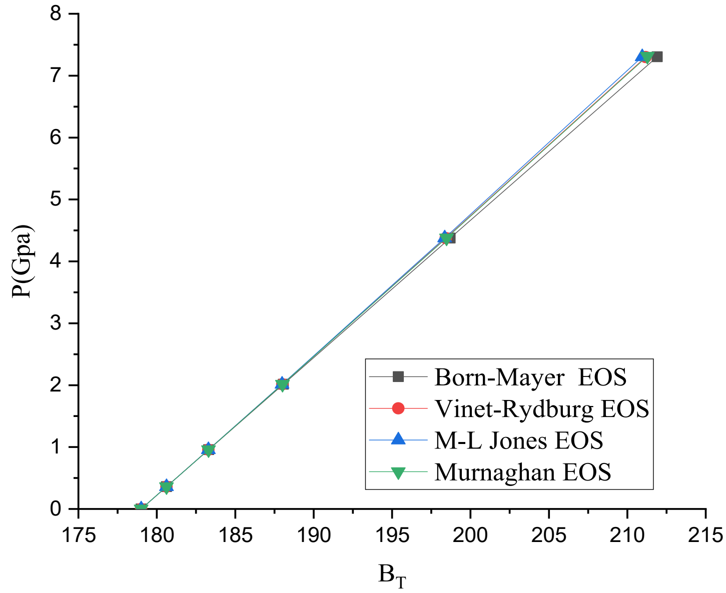
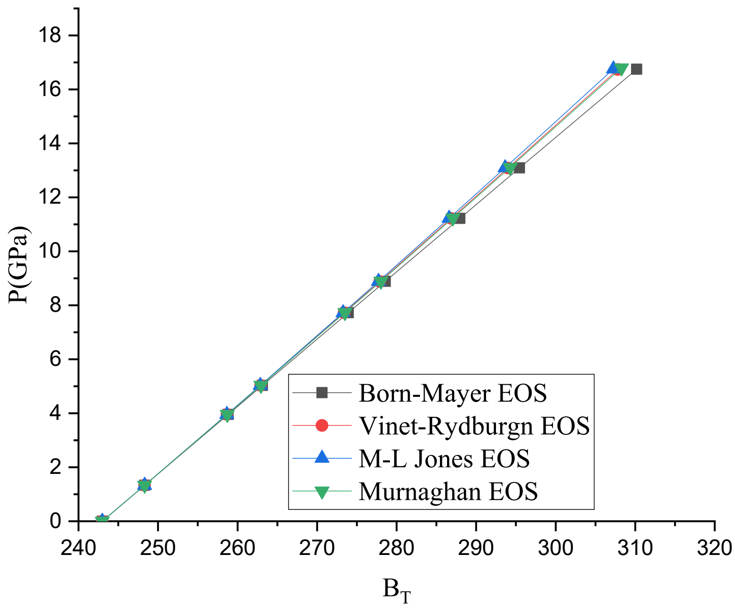


Fig-4: Variation of bulk modulus (B_T) at pressure (P) for nano TiO_2



From figure (3-4) it is clear that an increase in the isothermal bulk modulus (B_T) with pressure increasing results in higher pressure values across TiO_2 and nano-TiO_2. For TiO2, all four EOS exhibit good agreement at B_T range =190

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e-ISSN: 2468-4376
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GPa at 3 GPa pressure range; all four EOSs show significant differences in the B_T range. Similarly, in the case of nano-TiO_2, all four EOS exhibit good agreement at B_T range =275 GPa at 8 GPa pressure range; all four EOSs show significant differences in the B_T range.

A graph plotted between relative isothermal expansion coefficient under high pressure for TiO_2 and Nano-TiO_2

Fig-5: Variation of Relative isothermal expansion coefficient (α_r) at high pressure (P) for TiO_2

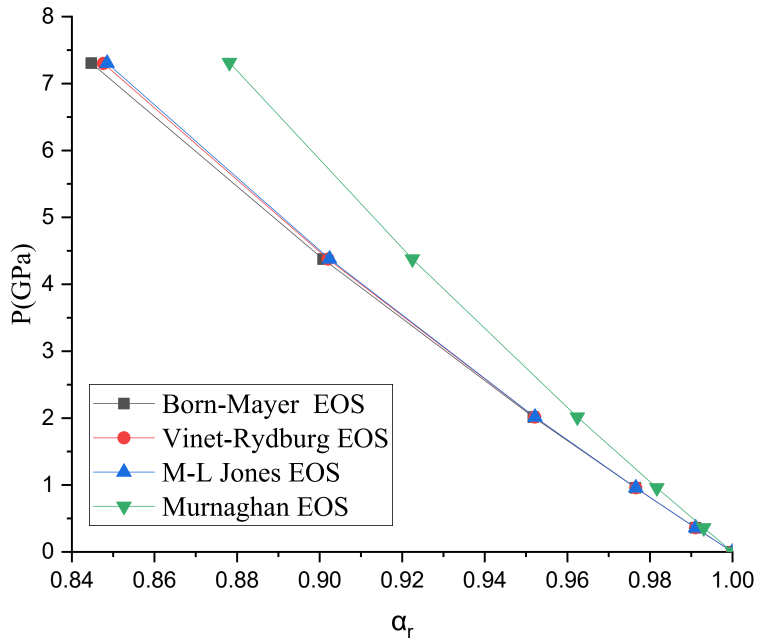
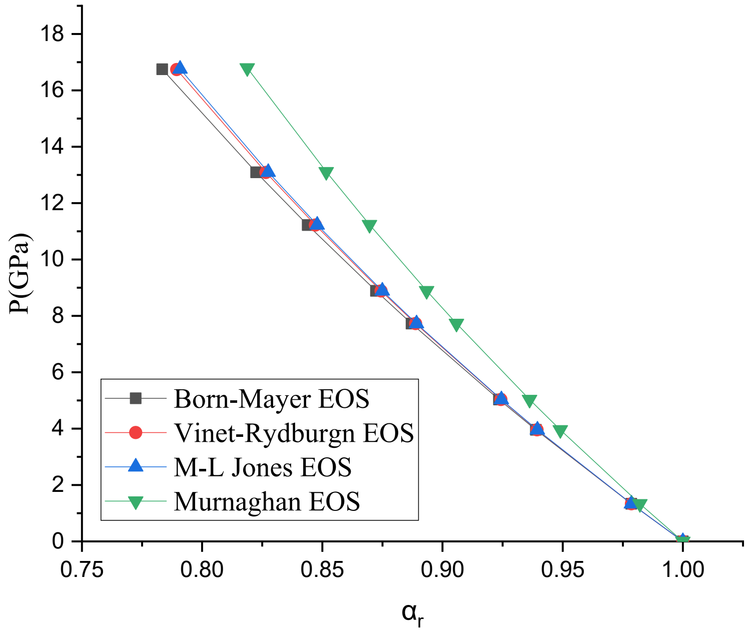


Fig-6: Variation of Relative isothermal expenssion coffecient (α_r) at high pressure for nano TiO_2



From figure (5-6) it is clear that the relative isothermal expansion coefficient increases with decreasing pressure for TiO_2 and nano-TiO_2. For TiO_2 all three EOSs (Vinet-Rydberg EOS, Born-Mayer EOS and M-L Jones EOS) exhibit good agreement with each other, but Murnaghan EOS shows slightly different results from the other three EOSs. Similarly, in the case of nano-TiO_2, all three EOSs (Vinet-Rydberg EOS, Born-Mayer EOS and M-L Jones EOS) exhibit good agreement with each other, but Murnaghan EOS shows slightly different results from the other three EOSs.

CONCLUSION

The overall study of thermoelastic properties viz. Pressure at different compression, isothermal bulk modulus and relative isothermal expansion coefficient at high pressure for TiO_2 and nano-TiO_2 lead to the conclusion that as pressure increases, compression value increases uniformly across both TiO_2 and nano-TiO_2 materials. It highlights computed pressure shows good agreement with experimental pressure at different compressions. Further, isothermal bulk modulus (B_T) increases with pressure increasing, all EOSs shows good agreement with each other. Furthermore, relative isothermal expansion coefficient increases pressure decreasing, all EOSs shows good agreement with each other apart from Murnaghan EOS.

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