

Research Article

High-Pressure Calibration TiN Equation of State

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Abstract

High pressure is becoming an interesting area of research for originating vital properties in crystalline solids. In the present study, the pressure equation of the state of TiN was investigated by employing various equations of state (EoS) presented in the literature, such as Dodson EoS, Barden EOS, Birch-Murnaghan (B-M) EoS. The EoSs were processed to find the high-pressure effects on the characterizations of TiN such as volume compression ratio, bulk modulus B , Grüneisen parameter, and phonon frequency spectrum. It was shown that a gigantic pressure results in a significant reduction in the volume of the TiN material, and the volume compression ratio reduction, is almost the same for the existing equations of state and the comparative literature results up to a pressure of 80 GPa. The maximum pressure difference is observed to be 4.85 GPa. over the entire pressure of 120GPa. Increasing the bulk modulus with high pressure was expected by the present EoSs, and up to the pressure of about 60 GPa, all curves of bulk modulus are matched with each other. Eventually, a fair comparison has been made between the present results and the first principle approximation along with the generalized gradient approximation method in which a perfect agreement was observed. Finally, the feasibility of TiN EoS as a standard pressure calibration was demonstrated.

Keywords: Equation of state EOS; volume compression ratio V_p/V_0 ; Bulk modulus B ; Grüneisen parameter; phonon density of state

1. Introduction

High microhardness, chemical and thermal stability, and refractoriness are all characteristics of titanium nitride. TiN is used in many different ways, including as a component in specialized refractories and cermets, as a material for metal crucibles during anoxic casting, and as a precursor for wear-resistant and aesthetically pleasing "gold-like" coatings. Studies on the combustion of compacted titanium powder samples in nitrogen revealed that one of the main factors influencing the combustion is the nitrogen filtration velocity within the titanium. A common, less expensive, and purer source of titanium than titanium powders is titanium sponge [1]. Despite its contribution to a wide variety of advanced industries, Titanium nitride has the great benefit of being electro-conductive and chemically stable, making it possible to mill it using the electro-discharge machining (EDM) method [2].

Under atmospheric pressure, TiN has a crystalline structure of NaCl (B1) and it can undergo a phase transition from B1 structure to CsCl (B2) structure at 320Gpa [3]. Hence, extra high pressure can be applied to this crystal while maintaining its phase and without occurring structural transition. To determine the effect of high pressure on the TiN structure, numerous efforts have been made. Using generalized gradient approximation [1] high-pressure effects on lattice volume, Bulk modulus, and phonon density of state have been studied up to the pressure of 50Gpa. Using

diamond anvil cell and X-ray diffraction method the EoS and stability of this compound have been measured up to the pressure of nearly 70 GPa and temperature of 2700 K [4] and up to pressure of 94GPa [5]. Based on the first principle approximation, the elastic constants, Debye temperature, and bulk modulus of this material, were investigated at high temperatures as well as high pressures [6]. In theoretical modeling, thermodynamic properties such as the relative compression volume, and bulk modulus of TiN are studied at moderate pressures up to (0–6 GPa) and high temperatures up to 2000 K [7].

High-pressure effects have attracted the scientific community to use equations of state as a time and cost-effective method to determine various characterizations of solid crystalline under high pressures. Different equations of state have been employed to describe pressure effects on various properties of Nano-TiO₂ [8]. Using three different equations of state, high pressure inducing useful characterization in Monoclinic Sulfur (S β) for the treatment of scabies in dermatology has been studied in [9]. Various equations of state were used to calculate, the bulk modulus and spinodal pressure of C₆₀ under strong compression [10]. The impacts of high pressure on the structural stability and melting point of Mo₅SiB₂ were investigated by using the first-principles calculations.

In this study, the effects of high pressure on the titanium nitrite are presented. The calculations of some properties

such as compressibility (V_p/V_0), bulk modulus (B), Grüneisen parameter, and phonon density of state are included, by employing Dodson EOS, Bardeen EOS, and modified Birch-Murnaghan EoS. The purpose of using different EOSs is to compare their results with each other along with the results in the relevant published scientific research. Moreover, owing to the high value of the bulk modulus of TiN, the pressure - V_p/V_0 relationship employment as a standard calibration for measuring high pressure is investigated. The presented results are compared with peer-reviewed up-to-date publications using the first principle and generalized gradient approximation.

2. Equation of State (EoS) for Solid Materials

Equations of the state are the relationships between the thermodynamic variable, such as pressure, temperature, and volume. When the temperature is kept constant, the pressure-volume relations are termed the isothermal equation of state. Equations of state offer, a time and cost-effective method to determine various characterizations of solid crystalline under high pressures [8]. This study tests the validity of three different EoS to be applied to TiN material in determining various thermodynamic and thermo-elastic properties under strong compression. EOSs are classified as follows:

1- Dodson EOS

Based on two simple parameters (Dodson, 1987) [11] derived an empirical EOS that fits all metals, metal alloys, ionic crystals, as well as semiconductors. The equation is given by:

$$P_{Do} = \frac{27}{8} B_0 B_0'{}^2 \left[\begin{array}{l} (\eta)^{-2/3} - 1 + 4 \left(1 - \frac{2}{3B_0'} \right) \\ \times \left\{ 1 - (\eta)^{-1/3} - \frac{1}{6} \left(1 - \frac{2}{3B_0'} \right) \ln \eta \right\} \end{array} \right] \quad (1)$$

where P_{Do} refers to the pressure due to the Dodson EOS, B_0 is bulk modulus at ambient pressure, B_0' indicates the first pressure derivative of bulk modulus, and $\eta = \frac{V_p}{V_0}$, is the volume compression ratio.

2- Birch-Murnaghan (B-M) EOS

B-M is a well-known equation of state for describing the thermodynamic behavior of the solid phase under high pressures, which is derived based on the internal potential energy in the solid and the pressure derivative of this internal potential energy. The B-M EOS [9, 12] is expressed by:

$$P_{B-M} = \frac{3B_0}{2} \left[\eta^{-7/3} - \eta^{-5/3} \right] \left[1 + \frac{3}{4} (B_0' - 4) (\eta^{-2/3} - 1) \right] \quad (2)$$

where P_{B-M} refers to the pressure required to introduce the compression ratio η .

3- Bardeen EOS [13].

Has settlement from the interatomic potential function (Er):

$$E_r = \frac{a}{r^3} + \frac{b}{r^2} + \frac{c}{r} \quad (3)$$

where, (a , b , c) are constant values, and (r) is the position function. Hence, the Bardeen equation can be given as:

$$P_{Ba} = 3B_0 \left(\eta^{-5/3} - \eta^{-4/3} \right) \left[1 + \frac{3}{2} (B_0' - 3) \left(\eta^{-1/3} - 1 \right) \right] \quad (4)$$

where, $P_{Bard.}$ is pressure according to the Bardeen EoS. An advantage of studying equations of state appears from its correlation with bulk modulus (B), which allows deriving the pressure dependence of bulk modulus. The bulk modulus of a substance is the pressure applied on the substance to introduce a relative change or reduction in the volume of the material, which is mathematically defined by: $B = -\Delta P / (\Delta V / V)$. This equation is rearranged to get the form of eq.5:

$$B = -V \frac{\partial P}{\partial V} \quad (5)$$

Eq.5 is represented as a bulk modulus dependent on pressure. This indicates that the bulk modulus increases with increasing pressure or reduction in the volume of the unit cell of solid material. At a given temperature, experiments have shown that the bulk modulus depends on the compression produced in the material (Birch, 1986). When the lattice spacing is decreased as a result of high pressure leads to introduce a significant repulsive interatomic force against the external agent. Hence, the bulk modulus equivalent to each equation of state is derived with Eq. (5). To derive the bulk modulus under high pressure by using Dodson EOS and B-M EOS, eq.1 and eq.2 are derivatives with respect to volume to obtain eq.6 and eq.7 as in the following steps:

$$\frac{dP_{Do}}{dV} = \frac{27}{8} B_0 B_0'{}^2 \left[\begin{array}{l} \frac{-2}{3} \frac{V^{-2/3}}{V_0^{2/3}} + 4 \left(1 - \frac{2}{3B_0'} \right) \times \\ \left\{ \frac{1}{3} \frac{V^{-1/3}}{V_0^{1/3}} - \frac{1}{6} \left(1 - \frac{2}{3B_0'} \right) \frac{1}{V} \right\} \end{array} \right] \quad (6)$$

then becomes

$$\frac{dP_{Do}}{dV} = \frac{27}{8} B_0 B_0'{}^2 \left[\begin{array}{l} \frac{-2}{3} \frac{V^{-5/3}}{V_0^{2/3}} + 4 \left(1 - \frac{2}{3B_0'} \right) \times \\ \left\{ \frac{1}{3} \frac{V^{-4/3}}{V_0^{1/3}} - \frac{1}{6} \left(1 - \frac{2}{3B_0'} \right) \frac{1}{V} \right\} \end{array} \right] \quad (7)$$

Differentiation of Eq. 2:

$$\frac{dP_{B-M}}{dV} = \frac{3}{2} B_0 \left[\left(\frac{V_p}{V_0} \right)^{-7} - (\eta)^{-5/3} \right] \left[\frac{3}{4} (B_0' - 4) \left[\frac{-2}{3} \frac{V_p^{-5/3}}{V_0^{-2/3}} \right] \right] + \frac{3}{2} B_0 \left[\frac{-7}{3} \frac{V_p^{-10/3}}{V_0^{-7/3}} + \frac{5}{3} \frac{V_p^{-8/3}}{V_0^{-5/3}} \right] \left[1 + \frac{3}{4} (B_0' - 4) \left[\left(\frac{V_p}{V_0} \right)^{-2} - 1 \right] \right] \quad (8)$$

where $\frac{dP_{Do}}{dV}$ and are pressure derivatives of Dodson and B-M, EoS respectively. Then, substituting Eqs. (7 & 8) into the bulk modulus definition in Eq. 5, one can find the Dodson EoS and EoS in terms of isothermal bulk modulus, as shown in Eq. 9 and Eq. 10:

$$B_{Do} = \frac{27}{8} B_o B_o'^2 \left[\frac{2}{3} (\eta)^{\frac{-2}{3}} - 4 \left(1 - \frac{2}{3B_o'} \right) \times \left\{ \frac{1}{3} (\eta)^{\frac{-1}{3}} - \frac{1}{6} \left(1 - \frac{2}{3B_o'} \right) \right\} \right] \quad (9)$$

$$B_{B-M} = \frac{B_o}{2} \left[7\eta^{\frac{-7}{3}} - 5\eta^{\frac{-5}{3}} \right] + \frac{3}{8} B_o (B_o' - 4) \times \left(9\eta^{\frac{-9}{3}} - 14\eta^{\frac{-7}{3}} + 5\eta^{\frac{-5}{3}} \right) \quad (10)$$

where B_{B-M} denotes the bulk modulus as a function of relative volume/pressure, in terms of Dodson EoS and B-M EoS respectively.

By the same method, expressions for the bulk modulus under high pressure according to Bardeen can expressed:

$$B_{Ba} = 3B_o \left(\frac{5}{3} \eta^{\frac{-5}{3}} - \frac{4}{3} \eta^{\frac{-4}{3}} - (B_o' - 3) \times \left(5\eta^{\frac{-5}{3}} - 3\eta^{\frac{-4}{3}} - 2\eta^{\frac{-4}{3}} \right) \right) \quad (11)$$

Where, B_{Ba} , is the bulk modulus according to Bardeen EoS.

3. Phonon Lattice Vibration

Einstein presented a model for atomic harmonic motions of the crystalline solids, in which all atoms are vibrating independently to each other with the same frequency. On the other hand, the idea of the single frequency dominant is no longer valid after Debye modifies solid lattice vibration. In Debye's model, instead of a specific frequency, a wide range of atomic frequencies are possible, in such a way that the number of frequencies is equal to the total degree of the freedom of the solid. The particles do not oscillate independently, but the vibrational motion of an atom does interact with its neighbors, and so on. Hence there is a band (spectrum) of frequency ranging from w to $w + dw$. The quanta of lattice vibration are referred to as phonons or modes of vibration, in which the number of active modes in the spectrum is termed as the density of state $g(w)$. In the Grüneisen theory [14, 15], the vibrational frequency of modes varies with the volume V of the unit cell, via Eq. 12 :

$$\gamma_i = - \frac{\partial \ln \omega_i}{\partial \ln V} \quad (12)$$

where denotes the Grüneisen parameter, ω_i is the frequency of the i^{th} mode of vibration, which is dependent on the lattice volume that is altered when high pressure is applied to the crystalline solid. Hence, the characteristics of the phonons

are dependent on the volume of the atomic unit cell because of the lattice an- harmonic behavior of the crystal. High pressure transforms the phonon energy into higher energy levels, as well as reduces the number of modes that acquire those high energy levels [16]. Consequently, the pressure dependence of both phonon frequency spectrum and density of the states are described by [12, 17]:

$$\omega = \omega_0 \eta^{-\gamma} \quad (13)$$

$$D(\omega, V_p) = D(\omega_0, V_0) \eta^\gamma \quad (14)$$

where, ω_0 and ω are the lattice frequency at atmospheric pressure and high-pressure P respectively. $D(\omega_0, V_0)$ and are respectively representing the density of states (modes) at zero pressure and high pressure. However, γ varies very slowly, and it is considered to be pressure-dependent. According to the following equation.

$$\gamma = \gamma_o \eta \quad (15)$$

Where, γ_o and γ stands for the Grüneisen parameter at zero pressure and high pressure respectively. The pressure dependence γ is due to the lattice an-harmonic behavior of crystalline [18]. Various methods were proposed for calculating the Grüneisen parameter at ambient conditions for various metals and alloys. For instance, the Grüneisen parameter can be calculated from the first pressure derivative of bulk modulus by the following relationships [19]:

$$\gamma = \frac{1}{2} \frac{dB}{dP} - 0.9 \quad (16)$$

4. Result and Discussion

In the present work, the high-pressure effect on the various properties of TiN such as unit cell volume V_p , Bulk modulus B , vibrational Grüneisen parameter γ , and phonon frequency spectrum is considered to be studied by employing three equations of state EoSs. The constant parameters used in this study are ($B_o = 281$ GPa, $B_o' = 4.46$) [20]. Figure 1 illustrates the variation of volume compression ratio from 1 to 0.78 at various high pressures for TiN, by using Dodson, Barden, and B-M EoS. It is clear that up to pressure, 80 GPa no real differentiation between the results of the three EoSs is observed. A comparable result with very little slope is seen at the lowest data of V_p/V_o which is 0.78. The present result of V_p/V_o attained with the EOSs is motivated to be compared with peer publication [1, 6], in which the first principle approximation method was used to estimate V_p/V_o of TiN up to pressure around 50 GPa and 60 GPa. It is shown that simulated results in [1, 6] are in very good agreement with the presented results obtained by the three considered EoSs. The marginal difference between the results of EoSs along with the presented findings in the literature, is due to the presence of a high bulk modulus of TiN, which is measured at 1281.6 GPa and its first pressure derivative of 4.46.

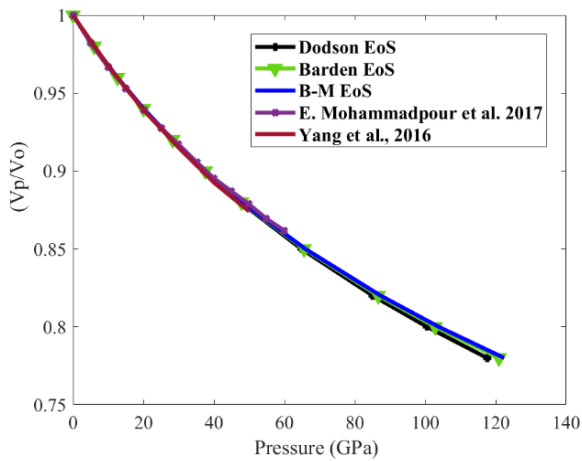


Figure 1. Compatibility of TiN, obtained with the present EoS, in comparison with Yang et al., 2016 [1] and E. Mohammadpour et al., 2017 [6].

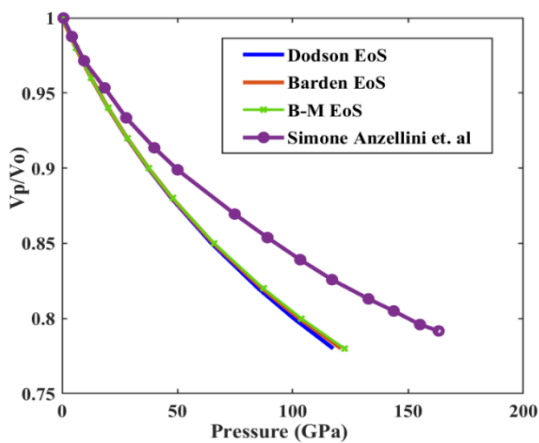


Figure 2. Comparison of the compressibility of TiN with Rhenium as measured by Simone et al., [21].

Furthermore, Figure 2 shows the comparison between the EoS of TiN and the EoS of Rhenium. It can be seen that Rhenium exhibits a lower compressibility than that of TiN under the same pressure. The low compressibility of Rhenium is due to its large ambient bulk modulus value. The bulk modulus of solid materials tends to increase under the application of high pressure. The lattice contraction resulting from the high pressure leads to the enhancement of the electrical repulsive force between neighboring particles which consequently increases the crystal resistance against the external pressure. Thus the increment in the bulk modulus has been proved in experimental as well as theoretical studies [6]. A remarkable outcome of the EoSs is the deduction of the pressure dependence of the bulk modulus which was given in Eqs. 7-9. The proposed EoSs give bulk modulus formulas that increase with increasing pressure and fit the experimental and theoretical observations. The variation in the value of bulk modulus with high pressure for TiN, calculated with the proposed EoSs along with peer publication investigation is depicted in Figure 3. The bulk modulus rose with increasing pressure from 280 GPa at ambient conditions, to up to 770 GPa at high pressure of 130 GPa with maintaining the relative volume of 0.78. However, all the results give a roughly equal value of B up to the pressure of 50 GPa, beyond this pressure limit the bulk modulus of Dodson EoS starts to diverge from the other results, demonstrating a difference of 70 GPa at the highest pressure of about 130 GPa. Table 1 represents a

statistical description of the results given in Figure 1 and Figure 3. Three volume compression ratio data (0.861, 0.84, and 0.80) are taken, and the pressure corresponding to each data is computed by the existing EoSs along with literature data. The averages of the pressures obtained by the three EoSs are found to be (58.61 GPa, 72.0239 GPa, 102.356 GPa). The standard deviation of the result of each EOS from the mean as well as the literature deviation from the mean are tabulated. It is shown that the standard deviation of the EoSs is increased with pressure (0.44, 0.614 and 2.95) GPa. Moreover, the bulk modulus at a high pressure of 59 GPa was calculated with each EoS, and the literature data are presented. The mean bulk modulus and the standard deviation are 493.9 GPa and 45.64 GPa respectively. The literature deviation from the mean bulk modulus of the EoSs is 41.85 GPa, which accounts for 8.47%.

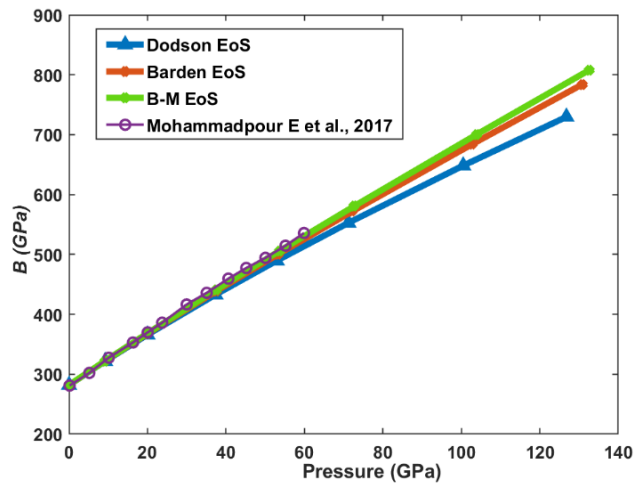


Figure 3. Bulk modulus as a function of pressure, calculated in the present study and compared with Mohammadpour E et al., [6].

The effect of high pressure on the Grüneisen parameter γ is of great importance due to its high relevance to the phonon frequency spectrum and density of states.

In the current contribution the γ at ambient state is found by substituting the first pressure derivatives of bulk modulus ($B'_0 = 4.46$) [6, 20] into Eq. 15, to get γ at zero pressure which equals 1.33. Then by combining the computed Vp/Vo data in Figure 1 into Eq.14, the Grüneisen parameter at various pressures is computed and shown in Figure 4. It can be seen that a very slight reduction in the Grüneisen parameter from 1.33 at ambient pressure to around 1.006 at a high pressure of 130 GPa is recorded by the three EoSs, with a negligible difference between the three data predicted. This result confirms the high lattice harmonicity of the TiN crystal up to a high-pressure range. The calculation of TiN, at zero pressure and its pressure dependence is considered as an initiative study.

The phonon frequency spectrum and density of states of TiN at atmospheric pressure were measured by [1] and the same phonon density of state was also investigated under high pressure of 50 GPa. In the current contribution, by combining the equations 12-14 with Vp/Vo data in Figure 1 and γ data in Figure 4, the phonon frequency spectrum and density of states under 50 GPa, by the three EoSs are displaced in Figure 4, and a comparative literature data is presented [1]. Due to the high bulk modulus of TiN, the curves of the proposed EoSs are matched to each other,

Table 1. Shows the statistic of deviation of the results obtained with the different equations of state and the comparative literature [6]

V_p/V_o	EoS	Pressure (Gpa)	Mean Pressure of the EoSs	Statistics		
				literature deviation from the mean	Standard deviation from the mean	
0.861	- Dodson	58.12	58.61 GPa	P mean=1.28 GPa	0.44 GPa	
	- Barden	58.72				
	- B-M	58.98				
	- Literature	59.89				
0.84	- Dodson	71.2134	72.023 9 GPa		0.614 GPa	
	- Barden	72.2084				
	- B-M	72.6501				
0.80	- Dodson	100.4744	102.356 GPa		2.95 GPa	
	- Barden	102.7867				
	- B-M	103.8077				
B		Pressure	B of EoS	Mean	Literature deviation	Standard deviation
	Dodson EoS	59 GPa	514 GPa	493.9 GPa	41.85 GPa	45.64 GPa
	Barden EoS		525.7 GPa			
	B-M EoS		442 GPa			
	Literature		535.75 GPa			

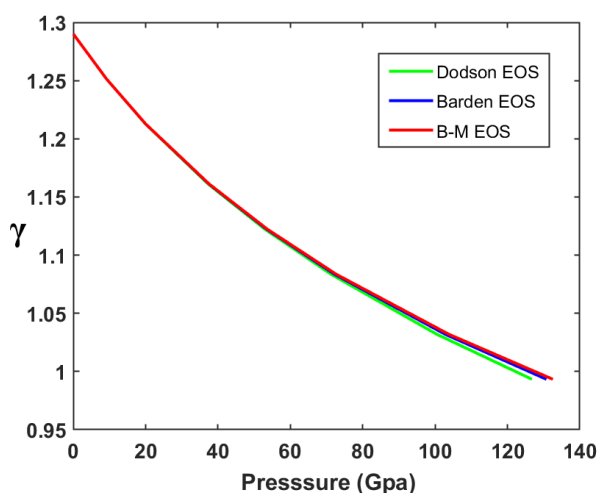


Figure 4. Variation of Grüneisen parameter with high pressure.

consequently, no substantial difference is observed. The phonon frequency spectrum shown in Figure 5 is comprised of two main bands of energy, the lower energy band is an acoustical mode and the higher energy band is the optical mode of the spectrum. Under the effect of high pressure, the optical spectrum is shifted towards higher energy. It is worth mentioning, that the high-pressure effect of the phonon

frequency spectrum measured in [1] by the first principle approximation, is in agreement with the present result by the above EOSs. Eventually, the comparative literature data along with the results of the existing EoSs, predict the same fact of the effects of high pressure on phonon density of state.

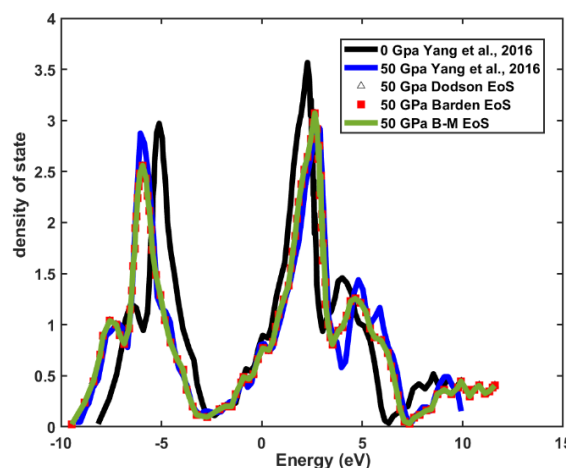


Figure 5. Phonon frequency spectrum and density of state of TiN, at zero pressure, and under 50 GPa calculated in the present study in comparison with [1].

It is worth mentioning, that the high-pressure effect of the phonon frequency spectrum measured in [1] by the first principle approximation, is in agreement with the present result by the above EOSs. Eventually, the comparative literature data along with the results of the existing EoSs, predict the same fact of the effects of high pressure on phonon density of state. The increase in the energy of the active modes in the present study completely fits the obtained result by [1], but there is a small discrepancy between the density of states at a pressure of 50 GPa. From the peak of the optical branch the density of state of the current study is greater by 0.152 from the presented literature data [1]. In contrast, from the acoustical band, the density of state calculated from the EoSs is lower than that recorded in [1] by 0.3157. At the ambient pressure, the total density of state $d(\omega)$ of the optical spectrum is 3.5, and the proposed EoSs predicted the reduction in this $d(\omega)$ by 14%, while in [1] the $d(\omega)$ is reduced by 0.6465 which equals 18% of the total density of state. To illustrate a higher transformation in energy and density of states, Figure 6 reflects the same fact, by measuring the phonon frequency spectrum and the density of states at 100 GPa by using Dodson EoS only. in comparison with the previous results. Under 100 GPa, a clear discrepancy between the results of the different curves is observed.

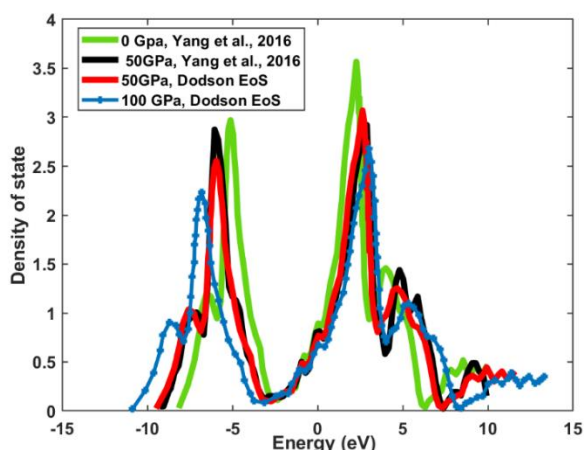


Figure 6. Phonon frequency spectrum and density of state of TiN, at zero pressure, and under 50GPa and 100GPa, calculated in the present study in comparison with, Yang et al. [1].

5. Conclusion

In the present three EoSs are proposed to determine the effect of high pressure on thermodynamic properties of TiN. The calculations included relative volume, Bulk modulus, Grüneisen parameter, and phonon density of state. However, these thermodynamic properties of TiN have already been determined by using first principle and generalized gradient approximation, this study was an initiative to test the feasibility of the EoSs to give results comparable with the peer publications. Due to the high compatibility (bulk modulus) of TiN, V_P/V_0 , B , and γ , all the EOSs gave roughly the same results up to 80 GPa. This indicates that the EoS of TiN using any of the considered EoS can be used as a fair pressure calibration method for other materials. According to our knowledge, the calculations of the Grüneisen parameter at ambient conditions, and its variation under high pressure can be a new contribution in the high-pressure research that can attract the scientific community. Eventually, the present results achieved with the considered EoSs demonstrated the same variation trend of the phonon

energy and density of states, as were predicted by the first principle approximation and the generalized gradient approximation in the literature results.

Nomenclature

TiN	Titanium nitride
GPa	Giga Pascal
K	Kelvin
η	Eta
V	Volume (cm ³)
P	Pressure (Gpa)
V_P/V_0	Volume compression ration
V_P	Volume under high pressure (cm ³)
V_0	Volume at ambient condition (cm ³)
γ	Grüneisen parameter

References:

- [1] R. Yang, C. Zhu, Q. Wei, and Z. Du, "Investigations on structural, elastic, thermodynamic and electronic properties of TiN, Ti₂N, and Ti₃N₂ under high pressure by first-principles," *Journal of Physics and Chemistry of Solids*, 98, 10-19, 2016.
- [2] J. Russias, S. Cardinal, J. Fontaine, G. Fantozzi, C. Esnouf, and K. Bienvenu, "Bulk titanium nitride material obtained from SHS starting powder: densification, mechanical characterization, and tribological approach," *International Journal of Refractory Metals and Hard Materials*, 23, no. 4-6, 344-349, 2005.
- [3] T.i Li, T. Liu, H. Wei, S.Hussain, B. Miao, W. Zeng, "Atomic and electronic structure of the TiN/MgO interface from first principles," *Computational Materials Science*, 105, 83-89, 2015.
- [4] K. Daviau, R. A. Fischer, M. C. Brennan, Junjie Dong, T. Suer, S. Couper, Y. Meng, V. B. Prakapenka., "Equation of state of TiN at high pressures and temperatures: A possible host for nitrogen in planetary mantles," *Journal of Geophysical Research: Solid Earth*, vol. 126, no. 2, p. e2020JB020074, 2021.
- [5] A. Dewaele, P. Loubeyre, and M. Mezouar, "Equations of state of six metals above 94 GPa," *Physical Review B*, 70, no. 9, 094112, 2004.
- [6] E. Mohammadpour, M. Altarawneh, J. Al-Nu'airat, Z.-T. Jiang, N. Mondinos, and B. Z. Dlugogorski, "Thermo-mechanical properties of cubic titanium nitride," *Molecular Simulation*, 44, 5, 415-423, 2018.
- [7] C. Dong, C. Jingdong, Z. Yinglu, Y. Benhai, W. Chunlei, and S. Deheng, "Theoretical study of the elastic properties of titanium nitride," *Acta Metallurgica Sinica (English Letters)*, 22, no. 2, 146-152, 2009.
- [8] A. I. Ghazal and A. M. Al-sheikh, "Thermo Elastic Properties of Nano-TiO₂ Under High Pressure Using Different Equations of State," in *Journal of Physics: Conference Series*, 1999, n1: IOP Publishing, 012075. 2021
- [9] R. ALSAQA and N. S. SULTAN, "Study of Thermodynamic Properties of Monoclinic Sulfur (β) Under High Pressure Using Three Different Equations of State for the Treatment Scabies in Dermatology," *International Journal of Thermodynamics*, 1-6. 2020.

- [10] A. Al-sheikh, S. Jalal, and R. Al-saqa, "Equation of state and thermo dynamic behaviour of C60 under high pressure, " *Universal Journal of Mechanical Engineering*, 8, , 59, 2020.
- [11] B. W. Dodson, "Universal scaling relations in compressibility of solids, " *Physical Review B*, 35, 6, p. 2619, 1987.
- [12] M. M. Tbeen, "Size Dependent Thermo Elastic Properties of Nano Lead Sulfide (PbS) under High Pressure, " *Rafidain Journal of Science*, 30, 12-20, 2021.
- [13] J. Bardeen, "Compressibilities of the alkali metals, " *The Journal of Chemical Physics*, 6, 372-378, 1938.
- [14] S. J. Al-Faris and S. K. Jalal, "Grüneisen Parameter Variation Consideration in Theoretical High-Pressure Studies for C60, " *Iranian Journal of Science and Technology, Transactions A: Science*, 46, 689-695, 2022.
- [15] R. H. Al-Saqa and S. J. Al-Taie, "Theoretical Study of Mechanical, Elastic and Phonon Frequency Spectrum Properties for GaAs at High Pressure, " *Журнал Сибирского федерального университета. Математика и физика*, 12, 371-378, 2019.
- [16] S. K. Jalal, A. M. Al-Sheikh, and R. H. Al-Saqa, "High pressure effects on the phonon frequency spectrum of silicon nanoparticle," *Iranian Journal of Science and Technology, Transactions A: Science*, 45, 391-396, 2021.
- [17] S. J. AL-FARÍS, R. H. Al-Saqa, H. M. MOHHAMED, and S. KAREEM, "High pressure effects on the structural properties of GaN compound using equations of state, " *International Journal of thermodynamics*, 25, 79-84, 2022.
- [18] A. ALSHEKH, S. KAREEM, and S. MAWLLOD, "Theoretical high-pressure study of phonon density of state and Debye temperature of solid C60: Grüneisen approximation approach, " *International Journal of Thermodynamics*, 25, 10-15, 2022.
- [19] N. Vočadlo and G. D. Price, "The Grüneisen parameter—computer calculations via lattice dynamics, " *Physics of the earth and planetary interiors*, 82, 261-270, 1994.
- [20] K. Prasert, P. Thanomngam, and K. Sarasamak, "First-Principles Investigation on Elastic Constants of TiN under High Pressure, " in *Advanced Materials Research*, 2013, 802: Trans Tech Publ, 109-113.
- [21] S. Anzellini, A. Dewaele, F. Occelli, P. Loubeyre, and M. Mezouar, "Equation of state of rhenium and application for ultra high-pressure calibration, " *Journal of Applied Physics*, 115, 043511, 2014.