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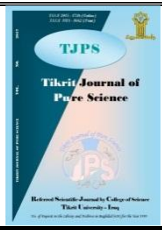

Study the change of some physical and chemical properties of TiN under high pressure

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ABSTRACT

The pressure equation of state of Titanium nitrate TiN was investigated in the current work using two equations of state (EOS) from the literature, including the Barden EOS and the Birch-Murnaghan EOS, whereas the Bardeen EOS, which is based on interstellar atomic potentials, and the Birch-Murnaghan EOS, which is based on the solid mechanics notion of finite strain. The EOSs were processed to identify the impacts of high pressure on the bulk modulus *B*, Debye temperature θ_D and lattice constant a, which are characterizations of TiN. Ultimately, a fair comparison of the current findings with the first principle approximation and the generalized gradient approximation approach was conducted, and a perfect agreement was found. It was demonstrated that TiN EOS can be used to calibrate high pressure for chemical compound TiN .

دراسة تغير بعض الخصائص الفيزيائية والكيميائية للمركب TiN تحت الضغط العالي

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الملخص

تم اختبار المعادلات العامة للحالة لنترات التيتانيوم TiN تحت الضغط العالي في هذا البحث باستخدام معادلتي الحالة (EOS) المستخدمة في عدة بحوث ومراجع عالمية، منها معادلتي باردين وبيرخ – مارنكهان (Barden and Birch-Murnaghan EOS) حيث أن معادلة باردين (Bardeen EOS) ، تعتمد على المجال والجهد الكهربائي الداخلي بين الذرات، اما معادلة بيرخ– مارنكهان (Birch-Murnaghan EOS)، فأنها تعتمد على الخصائص الميكانيكية للجهود الكهربائية للذرات. تم اختبار المعادلات اعلاه لتحديد تأثير الضغط العالي على معامل المرونة الحجمي B ودرجة حرارة دي باي θ_D Debye وثابت الشبكة a، والتي تمثل بعض الخصائص الفيزيائية والكيميائية للمركب TiN وتم إجراء مقارنة للنتائج التي تم الحصول عليها مع بعضها البعض من استخدام المعادلتين المذكورة اعلاه، حيث تم التوصل إلى توافق مثالي لكلا النتائج. لذلك توصلنا الى انه يمكن استخدام المعادلات اعلاه للحصول على نتائج تغير بعض الخصائص الفيزيائية والكيميائية للمركب TiN ومعايرتها تحت الضغط العالي دون الاجراءات العملية خاصة عند تعذر الحصول على قيم عالية من الضغط الهايدروستاتيكي.

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1. Introduction

TiN is one of the chemical element types that's found in the fourth group of the periodic table. Its ceramic has a tendency to resist corrosion. Spreading barriers is one of its uses, as is in some superconducting devices[1]. Due to TiN's useful characteristics, such as their high hardness, superior corrosion resistance, heat resistance, and great wear resistance, among others, titanium nitride (TiN) coatings have a wide range of uses [2]. Because of their hardness, high temperature characteristics, and wear resistance, nitrides are used in a wide variety of industries. Additionally, titanium nitride has the great benefit of being both electro-conductive and chemically stable, making it possible to mill it using the electro discharge machining (EDM) method, Ti has an atomic number of 22 and ends with the (s) shell by two electrons, but it will be paired with nitrogen, which will get an electron from the outer shell, to form a new series, and Ti is classified as a transition metal [3].

This study deals with the effect of high pressure on titanium nitrite, the calculation of some properties such as compressibility (v_p/v_o), bulk modules (B), lattice constant (a) and Debye temperature, by modified Birch-Murnaghan (B-M EOS) and Bardin-EOS, then compared the results of these equations where compared with the experimental results in the relevant published scientific research.

Where the Bardin EOS was applied to calculating the lattice constant at high pressure and the bulk modulus under high pressure for TiN. Then the (Barden and B-M EOS) were combined in order to see the difference in the results for the same variables, bulk modulus and phonon frequency, with high pressure, then the Barden EOS and B-M EOS were combined in order to see the difference in the results for the same variables, bulk modulus and phonon frequency, at high pressure.

2. Equation of state (EOS) for solid materials:

Two equations were employed in this study to get the required data. They are equations Birch-Murnaghan and Bardeen EOS. The premise of the (Birch-Murnaghan EOS), as it is known, is that when the temperature is constant, the bulk modulus of elasticity at any temperature varies as a linear function of pressure[3]. Ti, which is a metal with a hard, brittle, and high melting point that made it simple to consider it as an excellent metal for cutting tools and coating materials, was treated as a transition element in this research. Ti appears between group 1 and group 2 in the periodic table, which clarifies the reason for that reason. This explains why the atomic number of Ti is (22) and that it finishes with the (s) shell by two electrons.

This EOS is predicated on the idea that a solid undergoing compression can have its strain energy described as a Taylor series in limited strain[4].

$$P(V) = \frac{3}{2}B_o\left[\left(\frac{V_o}{V_P}\right)^{\frac{7}{3}} - \left(\frac{V_o}{V_P}\right)^{\frac{5}{3}}\right]\left\{1 - \left(\frac{3}{4}\right)(4 - B_o')\left[\left(\frac{V_o}{V_P}\right)^{\frac{2}{3}} - 1\right]\right\} \dots\dots\dots (1)$$

Where B_O bulk modulus at atmospheric pressure

$B`_0$:is the pressure bulk modulus derivative, or $B`_0 = \frac{dB_o}{dP}$

V_0 : is the volume at atmosphere pressure

Vp : is the volume at pressure P .

While Bardeen EOS had moved on from potential function (Er):

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

Where (a, b, c) are lattice constant values, and (r) is the position function, the Bardeen equation can be given as follows:[5]

$$P_{Ba} = 3B_o'\left(\eta^{-\frac{5}{3}} - \eta^{-\frac{4}{3}}\right)\left(1 + \frac{3}{2}(B_o' - 3)\left(\eta^{-\frac{1}{3}} - 1\right)\right) \dots\dots\dots (3)$$

$$\eta = \frac{V_p}{V_o}$$

3. The bulk modulus of elasticity:

It is the ratio between the bulk stress and the compliance stress. Its measured by the unit (Gpa), and can be cleared using the following equation: [6].

$$B = -V\frac{\partial P}{\partial V} \dots\dots\dots (4)$$

As the compliance stress is understood to be the ratio between the altered volume and its initial value, it is one unit less, and the negative sign denotes the decreased volume as the pressure rises.

4. Results and discussion:

4.1. Variations of bulk modulus under high pressure

Bulk modulus can be calculated mathematically under high pressure using data from table 1and according to the definition in equation (4)[7].

As we can use Birch-Murnaghan EOS and Bardeen EOS, then substitute them in equation (4) to get:

$$B_{B.M} = \frac{B_o}{2}\left[\frac{27}{4}(B_o' - 4)\left(\frac{V}{V_o}\right)^{-3} + \left(7 - \frac{21}{2}(B_o' - 4)\right)\left(\frac{V}{V_o}\right)^{\frac{-7}{3}} + 5\left(\frac{3}{4}(B_o' - 4) - 1\right)\left(\frac{V}{V_o}\right)^{\frac{-5}{3}}\right] \dots\dots\dots (5)$$

Table 1: parameters of TiN with its references

Ref.	Lattice constant a_o	Bulk modulus B_o	Derivative Bulk modulus B'	Gruneisen parameter	*Debye temp.*
[8]	4.23Å	271Gpa	4.3		
[1]				1.39	579 K

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4.2 Variation of lattice constant

The lattice constant variation has been studied for (TiN) with the pressure using the following equation [9].

$$a_p = a_o\left(1 + B_o'\frac{P}{B_o}\right)^{-\frac{1}{3B_o'}} \ldots\ldots\ldots\ldots\ldots(6)$$

Where a_p is the lattice constant at P (Kbar) pressure, $a_\circ$ lattice constant at atmospheric pressure.

As the values of the previous ratio $a_p = a_o\left(1 + B_o'\frac{P}{B_o}\right)^{-\frac{1}{3B_o'}}$ were used to determine the variation with pressure and apply Birch-Murnaghan EOS, they were offset in equation (6) to yield the figure(3). The theoretical results as calculations show the best agreement for both (Birch-Murnaghan and Bardeen EOS).

4.3 Calculation of Debye temperature for the TiN under the high pressure

The concept of Debye temperature has enormous importance in many fields and is known as the temperature at which the total average thermal energy is equal to a constant quantity as $\hbar w_D$.

Where; $\hbar = h/2\pi$, h: Blanks constant

w_D: is the cutoff frequency (Debye frequency), which is the highest frequency, and it's a constant quantity for all modes, longitudinal and transversal[10].

θ_D: is the Debye temperature; it's not the same for all materials, but changes according to the temperature and pressure [11,12].

$$\theta_{DP} = \theta_{Do}\left(\frac{V_o}{V_P}\right)^{\gamma} \ldots\ldots\ldots(7)$$

γ: First Grüneisen parameter at atmosphere pressure =1[13]..

θ_{Do}: Debye temperature at atmospheric pressure

θ_{DP}: Debye temperature at pressure (P).

Applying the last equation and considering (θ_{Do}=579 k) [14].

We extract the last figures (4) which represent the results of varying the Debye temperature with the press.

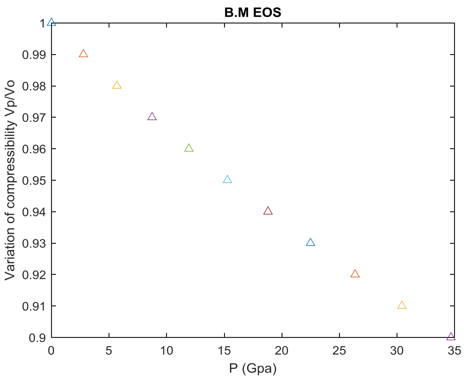

Fig. 1: Variation of compressibility with pressure using B-M EOS.

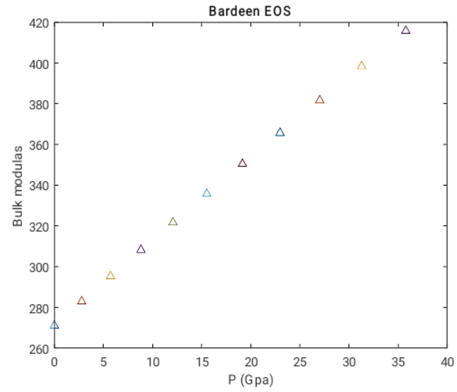

Fig.2a: Variation of Bulk modulus with pressure using Bardeen EOS.

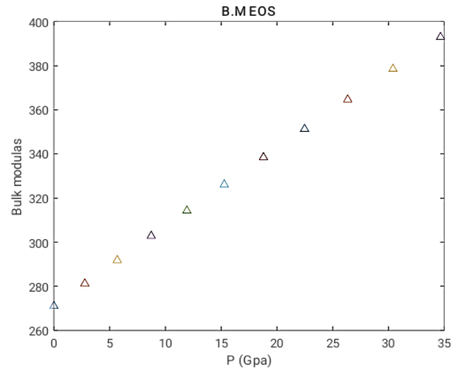

Fig. 2b: Variation of Bulk modulus with pressure Using B-M EOS.

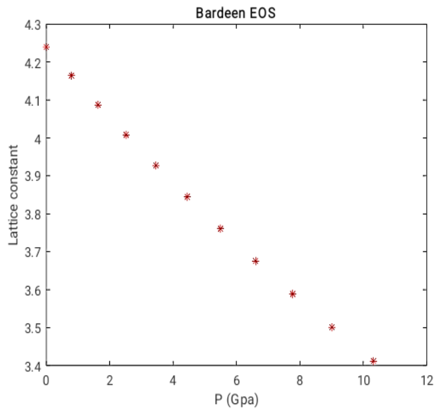

Fig. 3a: Variation of lattice constant with pressure Using Bardeen EOS.

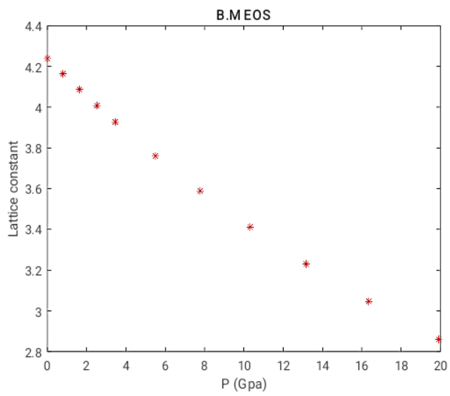

Fig. 3b: Variation of lattice constant with pressure using B-M EOS.

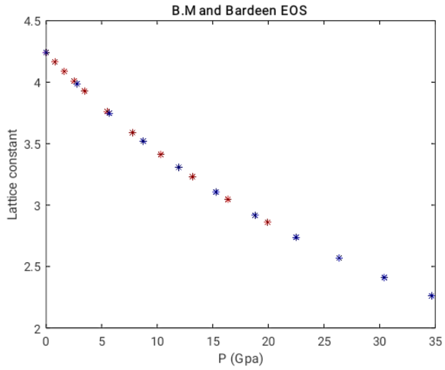

Fig. 3C: Comparing Variation of lattice constants with pressure using (Bardeen and B-M)EOSs

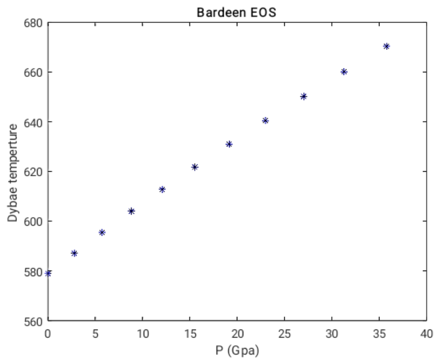

Fig. 4a: Variation of Debye temperature with pressure using Bardeen EOS.

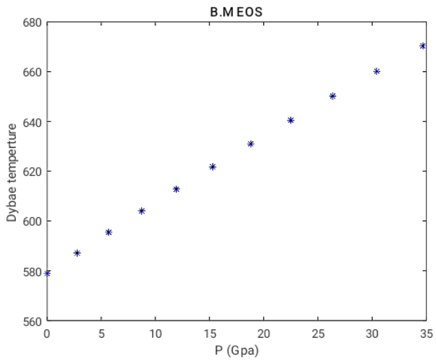

Fig. 4b: Variation of Debye temperature with pressure using B-M EOS.

5. Conclusion

From the data obtained by applying equations B-M and Bardeen, we get the results for all the parameters that we studied: bulk modulus, lattice constant, and Debye temperature under high pressure up to 35 Gpa. Using the two above equations, we obtained (figure. 1), compressibility, and lattice constant (figure.3), which are logarithmic proportional with pressure, whereas bulk modulus is directly proportional with pressure. The results show the agreement between the equations B-M and Bardeen EOS. The reason is that the material reaches a certain limit of contraction, and then stops compressing. The obtained results are in good agreement with the literature data [15,16], Then the suggestion is that all future studies for TiN under high pressure can be calculated by using one of the present equations of state (B-M and Bardeen) EOSs and can be used to calibrate for Tin parameters under high pressure.

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