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Study of Elastic Properties for Nano Sno_2 Under High Pressure Using Equations of State

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ABSTRACT

The current work examined the pressure equation of state of SnO_2 using two equations of state (EOS) from the literature: the Birch-Murnaghan (B-M) EOS and the Barden EOS. The latter is based on the solid mechanics concept of finite strain, while the former is based on interstellar atomic potentials. In order to determine the effects of high pressure on the bulk modulus B, and compaction volume , all of which are characteristics of SnO_2, the EOSs were processed. A perfect agreement was ultimately observed after a fair comparison of the current findings with the generalized gradient approximation approach and the first principle approximation. It was shown that pressure standards could be calibrated using SnO_2 EOS.

Keywords: *Bulk modulus, compression volume, lattice constant and Debye* temperature.

دراسة الخواص المرنة لثاني أكسيد الكبريت النانوي تحت ضغط عالٍ باستخدام معادلات الحالة

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ملخص

درس هذا العمل معادلة ضغط حالة أكسيد القصدير **(SnO2)** باستخدام معادلتي حالة **(EOS)** من المراجع العلمية: معادلتا حالة بيرش-مورناغان **(B-M)** وباردن. تعتمد الأخيرة على مفهوم ميكانيكا المواد الصلبة للإجهاد المحدود، بينما تعتمد الأولى على الجهد الذري بين النجوم. لتحديد آثار الضغط العالي على معامل الضغط الكلي **(B)** وحجم الضغط، وهما من خصائص أكسيد القصدير**(SnO2)** ، تمت معالجة معادلتي الحالة **(EOS).** لوحظ توافق تام بعد مقارنة دقيقة للنتائج الحالية مع نهج تقريب التدرج المعمم وتقريب المبدأ الأول. وقد تبين أنه يمكن معايرة معايير الضغط باستخدام معادلتا حالة أكسيد القصدير**(SnO2).**

الكلمات المفتاحية: معامل الضغط الكلي، حجم الضغط، ثابت الشبكة، ودرجة حرارة ديباي.

1.Introduction

Tin dioxide (SnO_2) is a wide-band gap semiconductor with applications in gas sensors, transparent conductive electrodes, and lithium-ion batteries [1]. At the nanoscale, SnO_2 exhibits unique mechanical, optical, and electronic properties due to quantum confinement and surface effects [2]. Understanding the elastic properties of nano SnO_2 under high pressure is essential for designing robust nanodevices. This study employs equations of state to model the pressure-dependent elastic behavior of nano SnO_2 [3]. Small crystallites with a diameter of 1–100 nm make up nanocrystals, which frequently exhibit unique physical and chemical characteristics that set them apart from their equivalent bulk materials [5]. One Nanoscale semiconductors, for instance, have electrical and optical

characteristics that vary with particle size, which makes them promising options for applications requiring electronic or optical property tunability.2, 3 From a fundamental perspective and in relation to the materials' potential applications, the question of how crystallite size affects structural stability in these nanocrystals is of great interest. In comparison to bulk materials, how would the relative stability of various potential solid structures alter for nanocrystals? Applying pressure to nanostructured materials to make them change from one solid structure to another is one method of answering this question. Tolbert and associates, the researchers [6-7], used surface-energy differences between the phases to explain why the transition pressure for the nanocrystals increased. Reduced grain size in PbS nanocrystals raises the transition pressure, according to Qadri et al.[8], whereas decreasing grain size enhances compressibility. In refrence [9], an increase in transition pressure was also noted. However, Jiang et al.[10] found that the phase transition pressure from α-Fe^2O_3 to γ-Fe_2O_3 is significantly lower for nanometer-sized γ-Fe_2O_3 particles than it is for bulk material. Bulk tin dioxide, or SnO_2, crystallizes in a rutile-type structure at ambient conditions [11].

The impact of high SnO_2 pressure is examined in this study. Using modified Birch-Murnaghan (B-M EOS) and Bardin-EOS, several properties were calculated, including compressibility (V/Vo) figures 1, bulk modules (B) figures 2, the outcomes of these three equations were then compared with the experimental findings in the pertinent published scientific research.

where the bulk modulus and lattice constant for SnO_2 under high pressure were determined using the Bardin EOS. In order to observe the difference in the outcomes for the identical variables, bulk modulus and V/Vo, with high pressure, the Barden and B-M EOS were then merged. In order to observe the differences in the outcomes for the identical variables, bulk modulus and V/Vo, at high pressure, the Barden EOS and B-M EOS were then merged.
In this study, Sn was considered a transition element. Sn is a metal that is hard, brittle, and has a high melting point, making it a great choice for cutting tools and coating materials. Its position in the periodic table between groups 1 and 2. This explains why Sn has an atomic number of 22 and possesses two electrons at the end of its (s) shell [12].

2. Solid material equation of state (EOS):

Two equations were utilized in this study to get the necessary data. (Birch-Murnaghan and Bardeen EOS) are these equations. The basis of the so-called Birch-Murnaghan EOS is that, at any temperature, the bulk modulus of elasticity varies as a linear function of pressure when the temperature remains constant [12]. The foundation of this EOS is the idea that a solid's strain energy under compression can be represented as a Taylor series in limited strain [13].

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

3.Equations of state

3.1. Bardeen EOS

Bardeen EOS had moved on from potential function (Er)[14].

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

The Bardeen equation can be expressed as follows when (r) is the position function and (a, b, and c) are constant values:

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

3. **The elastic bulk modulus:**

It is the proportion of compliance stress to bulk stress. The following formula can be used to clear it, and it is assessed in Gpa [15].

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

2.2. Vinet EOS

This equation is derived from "general inter-atomic potential" [16], and (Vinet et al) [17] derived it to be as:

$$\boldsymbol{P_V=3B_0\left(\frac{V}{V_0}\right)^{-\frac{2}{3}}\left[1-\left(\frac{V}{V_0}\right)^{\frac{1}{3}}\right]\exp\left[-3/2(B_0'-1)\left\{\left(\frac{V}{V_0}\right)^{\frac{1}{3}}-1\right\}\right]}\qquad(5)$$

4. Results and discussion

The aim of this research is to study nanomaterial properties "volume compression and bulk modulus" under high pressure using the EOS model. The two parameters " are listed in Table. 1, with its references, which are used to study volume compression and bulk modulus behavior under high pressure forSnO_2.

Table. 1: The input parameters used in the present work with the references

Nano materials	$\boldsymbol{B_0}$(GPa)	$\boldsymbol{B_0'}$	References
SnO_2	228	5.6	[18-19]

The variation of V/Vo was calculated under high pressure using deferent equation of state (B-M, Bardeen and Vinet EOS) and it illustrate in figure. 1, while the variation of bulk modulus evaluated using same equations, again it illustrated in figure 2.

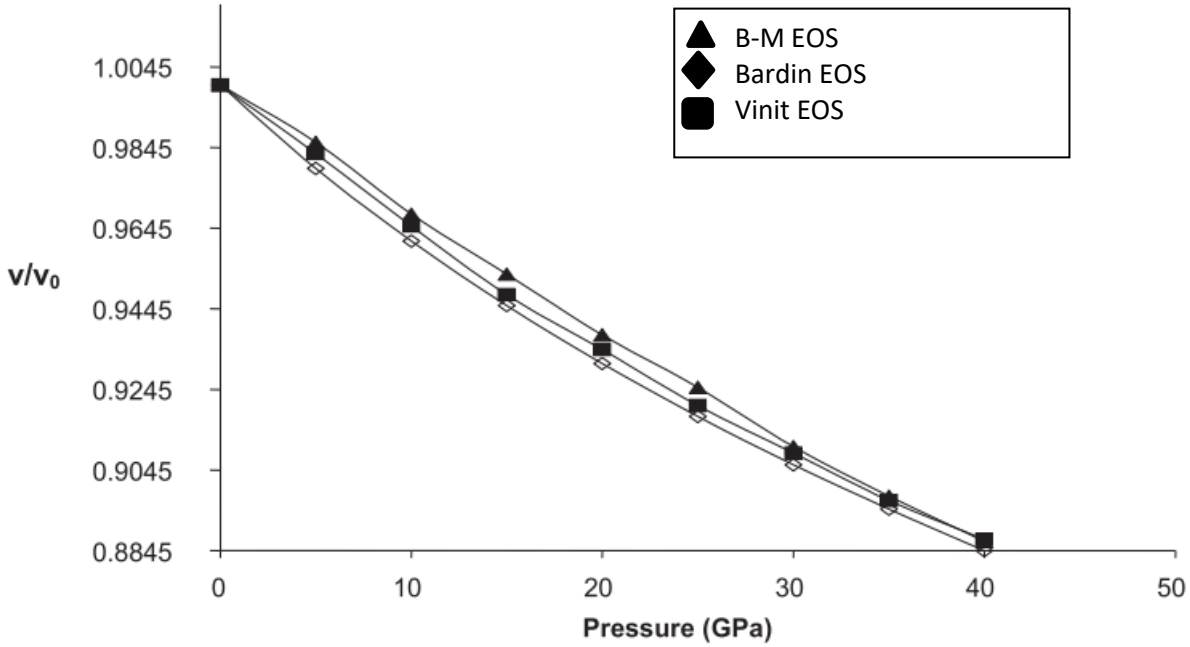

Figure.1: variation of volume comparison V/V_0 via pressure for SnO_2 using deferent EOS

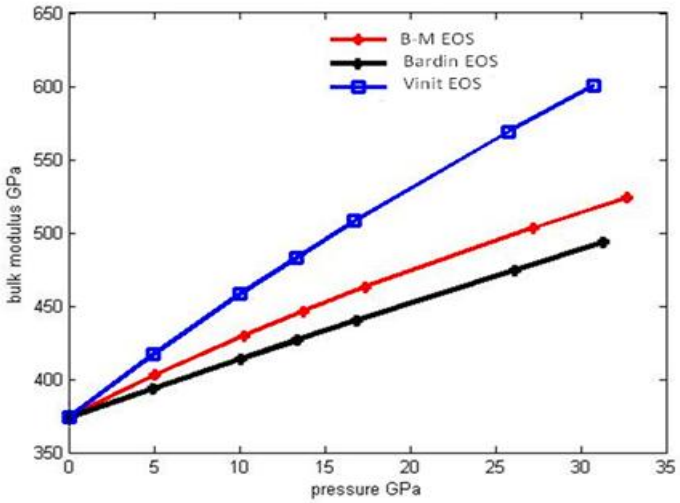

Figure 2. Variation of bulk modulus (B) with pressure for SnO_2 under high pressure

5. Conclusions

The compressibility and bulk modulus of the nanomaterial SiO_2 were calculated under high pressure up to 40 GPa, to protect the material from transforming into another phase after this high pressure value. The results showed that the Bardeen equation was more suitable than the Vinet equation and the B-M equations. This is because the Bardeen and Vinet equations depends on the mechanical properties of the material under atmospheric pressure, while the B-M equation and the Vinet equation depend on the interatomic potential. Therefore, the results of the Bardeen equation were more suitable and can be used in theoretical calculations to obtain good results that are compatible with practical experimental calculations.

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