



Structural, elastic, mechanical and thermodynamic properties of Terbium oxide: First-principles investigations



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ABSTRACT

First-principles investigations of the Terbium oxide TbO are performed on structural, elastic, mechanical and thermodynamic properties. The investigations are accomplished by employing full potential augmented plane wave FP-LAPW method framed within density functional theory DFT as implemented in the WIEN2k package. The exchange-correlation energy functional, a part of the total energy functional, is treated through Perdew Burke Ernzerhof scheme of the Generalized Gradient Approximation PBEGGA. The calculations of the ground state structural parameters, like lattice constants a_0 , bulk moduli B and their pressure derivative B' values, are done for the rock-salt RS, zinc-blende ZB, cesium chloride CsCl, wurtzite WZ and nickel arsenide NiAs polymorphs of the TbO compound. The elastic constants (C_{11} , C_{12} , C_{13} , C_{33} , and C_{44}) and mechanical properties (Young's modulus Y , Shear modulus S , Poisson's ratio σ , Anisotropic ratio A and compressibility β), were also calculated to comprehend its potential for valuable applications. From our calculations, the RS phase of TbO compound was found strongest one mechanically amongst the studied cubic structures whereas from hexagonal phases, the NiAs type structure was found stronger than WZ phase of the TbO. To analyze the ductility of the different structures of the TbO, Pugh's rule (B/S_H) and Cauchy pressure ($C_{12}-C_{44}$) approaches are used. It was found that ZB, CsCl and WZ type structures of the TbO were of ductile nature with the obvious dominance of the ionic bonding while RS and NiAs structures exhibited brittle nature with the covalent bonding dominance. Moreover, Debye temperature was calculated for both cubic and hexagonal structures of TbO in question by averaging the computed sound velocities.

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Introduction

Rare earth metals (REM) are found in earth's crust including seventeen (fifteen from the lanthanide group and two are yttrium and scandium) elements. REM is playing an imperative role in many modern technologies like giant magnetostrictive energy conversion, magneto-optical information storages, and high-strength permanent magnets due to their distinctive properties of luminescent, magnetic and electrochemical [1,2]. Moreover, RE has enabled the technologies and products more efficient, durable and thermally stable alongside maintaining a high standard of liv-

ing and saving lives. Rare earth (RE) oxides is a class of the REM compounds that are gaining an increasing interest because of their potential use in sundry applications and can yield lasing wavelengths [3,4] that make them qualified in memory devices [5] and as a refractory and abrasive materials [6]. Moreover, they are used as an improved efficiency phosphors and insulators in high-electric field devices [7–9].

Terbium (Tb) is one of the RE metals that has a hexagonal structure and a magnetocrystalline anisotropy characteristically for non zero orbital moments [10,11]. Tb possesses an oxidation number from +3 to +4, and forms oxides according to the general formula Tb_nO_{2n-2m} , depending on the procedure conditions. Recent measurements of the elastic constants and thermoelectric properties for different compounds have attracted the attention of many theoretical and experimental physicists because of a large amount of

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useful resulted information pertinent to the chemical bonding and the lattice dynamics [12–16].

Terbium monoxide (TbO), one of the oxide compounds of lanthanide group, and other lanthanide monoxide have been studied in non-magnetic RS structure [17]. Using the FP-LAPW method, Shafiq et al. (2015) investigated the elastic and mechanical properties of non-magnetic lanthanide monoxides, and predicated that these compounds are anisotropic and elastically stable. They also found that LaO, CeO, NdO, SmO, EuO, HoO and YbO were stiffer than the non-magnetic TbO. On the other hand, their calculations illustrated that the non-magnetic CeO, PrO, NdO, YbO, and TbO are ductile in nature.

Similarly, the structural, elastic and mechanical properties of the different RE oxides have recently been studied by many other researchers. Murtaza et al. (2015) calculated the elastic and thermoelectric properties of Mg_2X ($X = Si, Ge, Sn, Pb$) compounds by applying the FP-LAPW method, and they found that Mg_2Si and Mg_2Ge materials were isotropic and of brittle nature while Mg_2Pb and Mg_2Sn were found to be profoundly anisotropic and ductile [16]. Using first-principles calculations, Cheng et al. (2001) [18] studied the elastic properties and electronic structure of NiTi, CoTi, and FeTi. Zhao et al. [13] examined the structural and elastic properties and phase diagram as well of the NiTi alloy. Similarly, by employing the FP-LAPW method, Baltache et al. [19] analyzed the structural and elastic properties of the three alkaline earth oxides, namely MgO, CaO and SrO in RS structure. In cubic and orthorhombic phases, ab initio calculations were also performed to investigate the elastic, mechanical and thermo-acoustic properties of the ZrO_2 and HfO_2 . These compounds, possessing high bulk moduli, are considered very hard materials and are likely to display more ductility than brittleness [20]. In another study, the elastic constants of $ErVO_4$ were found noticeably smaller than those of isostructural silicate and phosphate analogs, indicating that these materials have potential applications as an interphase component in toughened oxide ceramic composites at room temperature [21].

The knowledge of the elastic properties gives a close view of the important characteristics of the solid such as inter-atomic potentials, the equation of state and phonon spectra which in turn are used to determine the Debye temperature, thermal expansion, specific heat, and the melting point of a material. Similarly, the bulk modulus (B), Young's modulus (Y), shear modulus (S) and Poisson's coefficient (σ), which measure the response of a crystal to external forces, can be dogged by using the calculated values of the elastic constants [20]. In addition, the bonding nature between adjacent planes of the atoms, determination of the crystal structural stability and the anisotropic character of the bonds is assessed by knowing elastic constants of a material [12].

Using the FP-LAPW scheme of calculations at the level of PBEGGA, first-principles spin-polarized calculations of TbO, crystallizing in RS, ZB, CsCl, WZ and NiAs types are performed to investigate the structural, elastic, bonding, mechanical, and thermal properties. To examine the ductility of the TbO in these different structures, we have calculated the elastic constants, B/S_H ratio, and the Cauchy's pressure. To the best of our knowledge, the elastic and mechanical properties of these TbO structures have not been reported previously. This paper is structured as follows: Section 2 is devoted to the method of calculation while Section 3 includes the results and discussion. The last section summarizes our findings.

Computational details

Reliability of the scheme of the calculations is crucial for scientific investigations particularly for unusual and quantum many body systems. Microscopic study of a typical solid material, con-

taining approximately 10^{23} atoms per cm^3 , is a quantum many-body problems. DFT based first-principles methods are intensively used to investigate the fundamental properties of the solid materials microscopically. Here we use the FP-LAPW (embodied in WIEN2k computational package) which is now considered as one of the most accurate DFT approaches [22]. In our calculations, the total energy calculations, to determine the ground state and elastic properties, are done at the level of the spin-polarized PBEGGA exchange-correlation functional [23] as PBEGGA is the most simple and reliable option for the treatment of the exchange-correlation energy functional [24,25], where the mechanical and thermodynamic properties were performed using IRelast package compatible with WIEN2k software's package [26]. The IRelast package is an ab initio tool to calculate the elastic constants of crystal structures with cubic symmetries. In this approach, calculations are done by taking "second-order derivative ($E''(\delta)$) of the polynomial fit of energy ($E = E(\delta)$) vs. strain at zero strain ($\delta = 0$)" [26]. Further details of the calculations concerning elastic constants for the cubic and hexagonal compounds as well as their allied properties can be consulted from the available literature [26–28].

In FP-LAPW approach, the unit cell is divided into atomic spheres and interstitial regions. In the both regions, to get adequate convergence, the basis functions were expanded up to $R_{MT} * K_M = 9$ in the unitcell where R_{MT} is the radius of the Muffin-tin spheres taken around atoms in the unit cell and K_M is the largest value of the k vector used for the plane wave expansion. Similarly, inside the atomic sphere, the maximum value of the $l_{max} = 10$ was used whilst the $G_{max} = 14$ was used for the Fourier expansion of charge density. The self-consistent convergence criteria of total energy calculations of the system are achieved when the total energy is stabilized within 10^{-5} Ry. The core states energy was separated from the valence states, at -6.0 Ry. Tetrahedron method was used to perform the integration over the Brillouin zone [29] by taking dense k-points mesh of $8 \times 8 \times 4$ for hexagonal and $8 \times 8 \times 8$ for the cubic structures. The simulated unit cell is optimized for total energy as a function of volume and the system was ensured at zero strain for its ground state. Then the obtained total energies are inserted to Murnaghan's equation of state [30] to find the ground state structural parameters/properties. In order to find the elastic properties, calculated elastic constants of the different TbO structures were fitted in the second-degree polynomial.

Results and discussion

Structural properties

The calculations were performed to determine the ground state properties for both cubic (rock salt (RS), zinc-blende (ZB), cesium chloride (CsCl)) and hexagonal (wurtzite (WZ) and nickel arsenide (NiAs)) polymorphs of TbO compound, using FP-LAPW method at the level of PBEGGA approximation. The bulk moduli and the corresponding values of pressure derivative have been computed, using Murnaghan's equation of state [30]. To increase precision, in the first step of these calculations, we optimized the lattice parameters for both cubic (rock salt (RS), zinc-blende (ZB), cesium chloride (CsCl)) and hexagonal (wurtzite and NiAs) phases. Then, the elastic constants were predicated by using the calculated optimized values of the lattice constants. The computed data for lattice constants (a_0), bulk moduli (B) and its pressure derivative (B) values, at minimum equilibrium volume V_0 , are presented in Table 1. These ground state properties of RS, ZB, CsCl phases of the TbO compound are obtained by following the approach given in Ref. [31]. Although the Table 1 show the comparison of the ground state properties of the different structures of TbO compound, no

Table 1

Structural parameters for the spin polarized RS, ZB, CsCl, WZ and NiAs structures which show the lattice parameters, bulk modulus, and its first derivative by using GGA approximation.

Structures	a(Å)	c(Å)	B(GPa)	B'
RS	4.8823	–	117.1762	4.9471
ZB	5.3212	–	91.5545	4.8378
CsCl	2.9823	–	122.8241	5.5147
WZ	3.7787	6.0890	88.1125	4.4559
NiAs	3.3769	6.0500	113.9801	5.4978

theoretical and experimental study is reported yet in literature for the comparison of ground state properties of the TbO compound.

Elastic properties

The calculations of the elastic constants are crucial because, through their knowledge, one can predict the response of a material to an applied macroscopic stress. In addition, the elastic parameters are essential for the understanding a variety of solid-state phenomena, for example, adjacent atomic planes bonding characteristics, structural stability, and anisotropic factor. The results of the elastic constants also play a key role in determining the mechanical properties like brittleness/ductility, stiffness, hardness. Our calculated values of the elastic constants in cubic (RS, ZB, and CsCl) and hexagonal (WZ and NiAs) structures at ambient pressure are listed in Table 2. By following the cubic symmetry, it is found, a cubic system needs only three independent elastic constants namely C_{11} , C_{12} and C_{44} for its complete description. However, for hexagonal crystal system, five independent elastic constants (C_{11} , C_{12} , C_{13} , C_{33} , and C_{44}) are required. As shown from Table 2, for all phases of TbO, the values of the calculated C_{ij} constants are positive. The generalized criterion for mechanically stable for a cubic system is as follows [32–34]:

$C_{11} > 0$, $C_{12} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$, $C_{11} > B > C_{12}$. From our results, for the cubic systems, the Born criteria for elastic stability are clearly satisfied, indicating that cubic TbO compound phases of interest are mechanically stable. Similarly, for hexagonal systems, criteria for mechanical stability [35] i.e. $C_{11} > |C_{12}|$, $C_{55} > 0$ is also found to be satisfied, showing that TbO wurtzite and NiAs structures are mechanically stable as well. Since no theoretical results are found in literature, we expect that our predictions can serve as a reference for further research on TbO.

Mechanical properties

From the calculations of the elastic constants, one can determine mechanical properties that include Young moduli (Y), Shear moduli (S), the anisotropic ratio (A), Poisson's ratio (σ), as well as compressibility (β) for RS, ZB, CsCl, WZ, and NiAs phases of the TbO (Table 3). To estimate these properties, foremost two schemes of approximations are typically used, that are Voigt (V) [36] and Reuss (R) [37,38]. In the Voigt assumption, for the polycrystalline materials, the aggregate strain corresponding to the external strain is considered uniform whilst in Reuss assumption,

the aggregate stress, for the polycrystalline materials, is considered uniform to the external stress. In addition, for the polycrystalline materials, elastic parameters are also estimated by employing Voigt-Reuss-Hill (VRH) approximation [39,40]. To determine the effective moduli results for the isotropic polycrystalline materials, following Hill expressions, in terms of the arithmetic mean, for Bulk and Shear's moduli are used:

$$B_H = 1/2 (B_V + B_R) \text{ and } S_H = 1/2 (S_V + S_R)$$

where the averaged compressibility is given by: $\beta = 1/B$.

The Hill Bulk modulus (B_H) and the Hill shear modulus (S_H) for the cubic system, which are related to the elastic constants, are given by, respectively,

$$B_H = \frac{1}{3}(C_{11} + 2C_{12}) \quad (1)$$

$$S_H = \frac{S_V + S_R}{2} \quad (2)$$

where $S_V = \frac{C_{11}-C_{12}+3C_{44}}{5}$ is the Voigt shear modulus and $S_R = \frac{5C_{44}(C_{11}-C_{12})}{4C_{44}+3(C_{11}-C_{12})}$ is termed as the Reuss shear modulus

While for the hexagonal systems, the B and S values in terms of the Voigt approximation are expressed as:

$$B_V = \left(\frac{1}{9}\right) \{2(C_{11} + C_{12}) + 4C_{13} + C_{33}\} \quad (3)$$

$$S_V = \left(\frac{1}{30}\right) \{C_{11} + C_{12} + 2C_{33} - 4C_{13} + 12C_{44} + 12C_{66}\}, \quad (4)$$

and in terms of the Reuss approximation as:

$$B_R = \{(C_{11} + C_{12})C_{33} - 2C_{12}^2\} / (C_{11} + C_{12} + 2C_{33} - 4C_{13}) \quad (5)$$

$$S_R = \frac{\left(\frac{5}{2}\right) \{[(C_{11} + C_{12})C_{33} - 2C_{12}^2]C_{55}C_{66}\}}{\left\{3B_V C_{55}C_{66} + [(C_{11} + C_{12})C_{33} - 2C_{12}^2]^2 (C_{55} + C_{66})\right\}} \quad (6)$$

The bulk modulus (B) measures the resistance offered by a material against changing its volume (hardness) or it represents the resistance to fracture. The shear modulus (S_H) describes the material's response to shearing strain or it represents the resistance to plastic deformation [37,39]. Their measurement is very important for engineering technological applications of a material.

The ratio of the stress to strain estimates Young's modulus (Y) which provides further information about the stiffness of a solid, that is, if the value of Y is higher, the material is the stiffer one.

By using Hill approximation, Y is given by:

$$Y = \frac{9BS_H}{3B + S_H} \quad (7)$$

The elastic anisotropic (A) is another fundamental parameter regarding mechanical properties. A is equal to one of an isotropic material. In a crystal, this parameter is the measurement of the anisotropy of the elastic wave velocity and is given by:

Table 2

Calculated elastic constants (C_{ij} , in GPa) of the TbO compound in cubic (RS, ZB, and CsCl structures) and hexagonal (WZ and NiAs structures) systems at ambient pressure by using GGA approximation.

Elastic constants (GPa)	Cubic structures			Hexagonal structures	
	RS	ZB	CsCl	WZ	NiAs
C_{11}	190.84	107.89	300.65	148.80	228.41
C_{12}	78.43	86.21	33.17	59.78	32.59
$C_{44}=C_{55}$	103.25	57.85	15.73	33.45	89.06
C_{13}	–	–	–	49.77	44.54
C_{33}	–	–	–	146.40	312.68

Table 3
Calculated bulk (B_V , B_R , and B_H) and shear moduli (S_V , S_R , and S_H) in Voigt, Reuss and Voigt-Reuss-Hill approximations (in GPa), compressibility (β , in GPa^{-1}), Young modulus (Y , in GPa), Poisson's ratio (σ), B/S_H ratio, anisotropic factor A , Cauchy's pressure $C_{12} - C_{44}$ and Vickers hardness (H_V) for the cubic and hexagonal TbO compound in comparison with available experimental and theoretical data.

	Cubic structures			Hexagonal structures	
	RS	ZB	CsCl	WZ	NiAs
B_V	115.90	93.44	122.33	84.74	112.54
B_R	115.90	93.44	122.33	84.62	109.63
B_H	115.90	93.44	122.33	84.68	111.09
β	0.008628	0.010702	0.008174	0.011809	0.009001
S_V	84.43	39.04	62.93	41.26	98.39
S_R	77.35	21.16	24.31	40.13	96.94
S_H	80.89	30.10	43.62	40.69	97.66
Y_V	203.81	102.81	161.16	106.49	228.57
Y_R	189.83	59.02	68.39	103.95	224.61
Y_H	196.87	81.55	116.96	105.23	226.59
σ_V	0.206	.316	.280	.290	0.161
σ_R	0.227	.394	.406	.295	0.158
σ_H	0.216	.354	.340	.292	0.160
B/S_H	1.43	3.10	2.80	2.08	1.14
A	1.84	5.34	0.12	0.68	0.79
$C_{12} - C_{44}$	-24.82	28.36	17.44	26.33	-56.47
H_V	14.15	0.89	2.45	4.42	22.09

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \text{ for the cubic systems} \quad (8)$$

and

$$A = \frac{4C_{44}}{C_{11} + C_{33} - 2C_{13}} \text{ for the hexagonal systems} \quad (9)$$

The Poisson's ratio (σ) is given by the following relation

$$\sigma = \frac{3B - 2S_H}{2(3B + S_H)} \quad (10)$$

Based on the elastic properties of the different phases of the TbO, the calculated physical and mechanical properties of the corresponding structures are analyzed as follows:

Hardness, a macroscopic concept, is characterized by how much the material is resistant to change in its shape and thus depending strongly on plastic deformation [38,41]. Often used as preliminary predictors, bulk modulus (B) measures the opposition offered against the volume change in the company of inflexible magnitude whereas shear modulus (S) is the measurement of the resistance offered against the shear deformation [38,40,42,43]. Following are the ways, with which the hardness of a material is represented: (i) bulk modulus (ii) shear modulus and (iii) Vickers hardness (computed as $H_V = 2(k^2S)^{0.585} - 3$ where $k = S/B$; B : bulk modulus) and S : shear [44]. Although hardness is better predicted by shear modulus as compared to bulk modulus [45], in recent research Chen et al. has shown that Vicker approach demonstrates better hardness than shear modulus [44]. As it can be seen from the Table 3, for all of the examined systems, the value of the bulk modulus B is found greater than the shear modulus. This implies that the parameter limiting the mechanical stability of these structures is the shear modulus. In the cubic system, Bulk moduli results predict that CsCl type phase of TbO is the hardest one since it has the higher value of it. In contrast, shear modulus and Vickers hardness calculations predict that RS TbO is the hardest structure from all other studied structures. Table 3 shows in hexagonal system, the shear modulus and bulk modulus of NiAs type structure are superior to WZ of the TbO indicating that NiAs type TbO is harder than WZ TbO as consistent with the computed results of the Vickers hardness, using Hill's data. On the other hand, the compressibility β , which is related to elastic deformation [38,41] in the structures of the cubic system, has the minimal value for CsCl and RS type structures while NiAs type structure has the minimal value in the hexagonal system. This reveals that these phases of the TbO

are more stable and less compressible against the external deformation.

Stiffness is described by a resistance force against distortion. Young's modulus, calculated via stress to strain ratio, is considered to find out the stiffness level of a material. According to this definition, if the value of Y is larger, the material is considered to be stiffer. Our calculated Hill's Young's modulus, in Table 3, indicates that RS TbO is the stiffest phase among other investigated cubic structures, as RS TbO have the largest values of elastic constants from the all cubic structures in question. This means that RS structure of TbO is mechanically the strongest among all cubic phases. Similarly, the NiAs structure of TbO has larger Hill's Young's modulus than WZ structure, indicating that NiAs is stiffer than wurtzite in the hexagonal system. Since the elastic constants of the NiAs structure of TbO are larger than those of the WZ structure of TbO, the NiAs TbO is mechanically stronger than WZ TbO. Furthermore, the types of bonding in a solid can be predicted by knowing the sign of Cauchy pressure ($C_{12} - C_{44}$). The sign of the Cauchy pressure of the dominant covalently bonded compounds is negative while it is positive for the compounds with dominant ionic bonds [45]. An added indicator which can be used for the bond sorting is a value of the Poisson's ratio. For a typical covalently bonded compound, the value of the Poisson ratio is too lower than 0.25 while that of a typical ionic compound, it is nearly 0.25 or more [46]. The Cauchy pressure ($C_{12} - C_{44} > 0$) results predict that in the ZB structure of TbO, ionic bonds dominant than the CsCl structure of TbO. On the other hand, the Cauchy pressure ($C_{12} - C_{44} < 0$) predicts that for RS structure of TbO, covalent bonds are dominant. In contrast, in the hexagonal system, our sign of Cauchy pressure ($C_{12} - C_{55}$, for hexagonal structures $C_{44} = C_{55}$) foretells that for WZ structure, ionic bonds are dominant whereas in NiAs TbO covalent bonds are dominant. Our calculations show that Poisson's ratios are $\sigma_H = 0.354$, 0.340 and 0.216 for ZB, CsCl, and RS TbO, respectively. Poisson's ratios, however, are $\sigma_H = 0.292$ and 0.160 for WZ and NiAs TbO, respectively as can be seen from Table 3. Therefore, by following the trend of the values of the Poisson's ratio, ZB, CsCl and WZ structures of TbO exhibit ionic bonds but RS and NiAs structures of TbO are with covalent bonds. In fact, these results are consistent with the predicted results by the Cauchy pressure sign as well. Thus we note that RS and NiAs are the stiffest material among the studied structures and have covalent bonds as well.

One more key mechanical feature of the materials is the brittle/ductile behavior. In this context, the widely used measure

Table 4

The calculated values of density (ρ in g/cm³), the sound velocity of transverse v_t , longitudinal, and average sound elastic wave velocities v_m , Debye Temperature (θ_D) in K) of TbO compound.

Structure	ρ (g/cm ³)	v_t (m/s)	v_l (m/s)	v_m (m/s)	θ_D (K)
RS	9.9838	2846.48	4734.15	3148.25	383.961
ZB	7.7115	1975.73	4161.85	2222.7	248.722
CsCl	10.8318	2006.72	4082.06	2253.36	282.391
WZ	7.7077	2297.75	4245.71	2564.23	286.893
NiAs	9.7135	3170.87	4984.19	3486.13	421.298

is the Pugh's indicator (B_H/S_H) [47]. By following Pugh indicator [47], if $\frac{B_H}{S_H} < 1.75$, it means that a material is of brittle nature, and vice versa. On the other hand, if $\frac{B_H}{S_H} > 1.75$, a material would act as ductile [45]. Our results show that the ($\frac{B_H}{S_H}$) ratio for RS, ZB, and CsCl TbO are 1.43, 3.10 and 2.80, respectively. This means that RS TbO is brittle but ZB and CsCl structures of TbO are ductile, taking into consideration that ZB phase of TbO is more ductile than CsCl phase in the cubic system. However, in the hexagonal system, $\frac{B_H}{S_H}$ the ratio for WZ TbO and NiAs are 2.08 and 1.14, respectively. This suggests WZ TbO is ductile while NiAs TbO is brittle (see Table 3).

Another important parameter that correlates with the possibility of microcracks appearance in materials is the elastic anisotropy of crystals [48]. The elastic anisotropy of the crystals is represented by different ways, among one of them is done by using the calculated values of the C_{ij} constants. A measure of the degree of anisotropy in the bonding between atoms in different planes can be known by calculating the shear anisotropic factors [49,50], especially for the {100} shear planes between $\langle 011 \rangle$ and $\langle 010 \rangle$ directions. For crystals with isotropic elastic properties $A = 1$, or smaller or greater than unity, measure the degree of elastic anisotropy. In our case, as Table 3 shows, the calculated anisotropic ratio for all cubic structures of TbO deviates from 1. This shows that these phases of the TbO are not isotropic elastically and therefore, their properties are not elastically isotropic, meaning that in different directions their properties are different. Our calculated anisotropic ratio for the both phases (WZ and NiAs) somewhat deviates from unity, hence demonstrating isotropic conduct for these structures of TbO. Our calculated results for anisotropic factor A, as listed in Table 3, shows that the minimal anisotropy of the CsCl phase of the TbO among the examined structures of TbO compound.

Thermal properties

The assessment of upper and lower limits of the mechanical properties is signified by the Voigt and Reuss equations (VRe) [45]. Similarly, thermodynamic properties, for example, Debye temperature (θ_D) and average sound velocity (v_m) which is approximated by a relation involving the transversal (v_t) and longitudinal (v_l) sound velocities are also figured out within Hill scheme (the average of VRe).

Debye temperature (θ_D) a fundamental parameter, is very much correlated to several physical properties like elastic constants, melting temperature, specific heat etc. Moreover, thermal loss mechanisms called as the temperature dependence of a material is correctly depicted in term of θ_D . One of the typical ways to compute the Debye temperature is based on elastic constants values, because θ_D is predictable from the v_m by the following equation [51,52]:

$$\theta_D = \frac{h}{k_B} \left[\frac{3n}{4\pi} \left(\frac{N_A \rho}{M} \right) \right]^{1/3} v_m \quad (11)$$

where h is Plank's constant, k_B is Boltzmann's constant, N_A is Avogadro's number, n is the number of atoms per formula unit, ρ is

the density, M is the molecular weight and v_m is average sound velocity. The average sound velocity is approximately calculated from [52,53] as:

$$v_m = \left[\frac{1}{3} \left(\frac{2}{v_t^3} + \frac{1}{v_l^3} \right) \right]^{-1/3} \quad (12)$$

where v_t and v_l are the transverse and longitudinal sound velocities. These are obtained by using the shear modulus S and the bulk modulus B from Navier's equation [54] as:

$$v_l = \left(\frac{B + \frac{4S}{3}}{\rho} \right)^{1/2} \quad \text{and} \quad v_t = \left(\frac{S}{\rho} \right)^{1/2} \quad (13)$$

where ρ is the mass density per unit volume.

By using computed results of the elastic constants given in Table 2, we calculated v_t , v_l , v_m , θ_D and density for each phase of the TbO as presented in Table 4. One can note that mainly the sound velocities are dependent on the obtained results of the elastic moduli (Bulk modulus (B_0) and shear modulus (S)) of a material. It means that if a material has large values of the elastic moduli, correspondingly it will show a higher sound velocity. However, to our best knowledge, no measured data is available in the literature for comparison. Therefore, our presented results here can be considered, in both cubic and hexagonal structures, as a prediction concerning TbO compound properties. This study can be a reference for future experimental measurements.

Conclusions

First-principles calculation is performed to study the structural, elastic, mechanical and thermodynamic properties of the TbO compound in both cubic and hexagonal phases. To that end, calculations were performed using FP-LAPW scheme of calculations at the level of PBEGGA exchange-correlation energy functional. The optimized structural parameters like lattice constants, bulk moduli, and total energy for the each phase were obtained. The Born elastic stability conditions for both systems (cubic and hexagonal) are clearly satisfied by our results. Elastic constants of RS TbO has the largest values for all investigated cubic structures, the RS phase of TbO was found to be mechanically stronger among the cubic structures, whereas, for hexagonal structures, NiAs phase was found stronger than WZ phase of TbO. Shear modulus and Vickers hardness calculations also endorsed that RS phase of TbO was the hardest one from the cubic structures and NiAs phase of TbO was harder than WZ phase of TbO. The minimal values of the compressibility were for CsCl and RS phase of the cubic system and for NiAs phase of the hexagonal system. Our calculation of Young's modulus indicates that RS phase of TbO was the stiffest one from the cubic phases in question and NiAs was found to be stiffer than wurtzite phase in the hexagonal system. From the comparison of the value of Cauchy pressure ($C_{12} - C_{44}$) and Poisson's ratio, it was found that for the ZB, CsCl and WZ structures of TbO, the ionic bonding was dominant, while for RS and NiAs phases, the covalent bonding was dominant. The values of anisotropy constant for both cubic and hexagonal system deviated from unity. Our results show that

RS and NiAs phases of TbO compound were brittle in nature but ZB, CsCl and WZ phases of TbO were ductile. The sound velocities and Debye temperature were also calculated for these structures.

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