Structural, elastic, and electronic properties of topological insulators: Sb₂Te₃ and Bi₂Te₃

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Abstract— We have performed a first principles study of structural, elastic, and electronic properties of rhombohedral Sb₂Te₃ and Bi₂Te₃ compounds using the density functional theory within the local density approximation. The lattice parameters of considered compounds have been calculated. The second-order elastic constants have been calculated, and the other related quantities such as the Young's modulus, shear modulus, Poisson's ratio, anisotropy factor, sound velocities, and Debye temperature have also been estimated in the present work. The calculated electronic band structure shows that Sb₂Te₃ and Bi₂Te₃ compounds have a direct forbidden band gap. Our structural estimation and some other results are in agreement with the available experimental and theoretical data.

Keywords— *ab initio* calculation, mechanical properties, electronic structure

I. INTRODUCTION

Sb₂Te₃ and Bi₂Te₃, the members of compounds with the general formula $A_2^V B_3^{VI}$ ($A = \text{Bi, Sb}$ and $B = \text{S, Se, Te}$), are narrow-bandgap semiconductors with rhombohedral layered crystal structure. Sb₂Te₃ and Bi₂Te₃ are well-known topological insulators [1-7], extraordinary thermoelectric materials at ambient temperature [8] and the possible topological superconductors [9] with surface states consisting of a single Dirac cone at the high symmetry point $-\Gamma$. All of these have made $A_2^V B_3^{VI}$ compounds as the subject of intensive investigation both in fundamental and applied research. These compounds possess the rhombohedral crystal structure with five atoms per unit cell belonging to the space group $D_{3d}^5(R\bar{3}m)$. Sb₂Te₃ and Bi₂Te₃ can be used for many different applications such as power generation and cooling devices [10]. Thermoelectric power generators and cooler have many advantages over conventional refrigerators and power generators such as long life, no moving parts, no green house gases, no noise, low maintenance and high reliability [11-13].

As far as we know, no *ab initio* general potential calculations of the mechanical properties such as the shear modulus, Poisson's ratio, anisotropy factor, sound velocities, Debye temperature of the Bi₂Te₃ and mechanical properties of Sb₂Te₃ have been reported in detail. In the present work, we

have investigated the structural, electronic, and photon energy-dependent optical properties of the Sb₂Te₃ and Bi₂Te₃.

II. SIMULATION

Our calculations have been performed using the density functional formalism and local density approximation (LDA) [16] through the Ceperley and Alder functional [17] as parameterized by Perdew and Zunger [18] for the exchange-correlation energy in the SIESTA code [19, 20]. This code calculates the total energies and atomic forces using a linear combination of atomic orbitals as the basis set. The basis set is based on the finite range pseudoatomic orbitals (PAOs) of the Sankey_Niklewsky type [21], generalized to include multiple-zeta decays. The interactions between electrons and core ions are simulated with separable Troullier-Martins [22] norm-conserving pseudopotentials. We have generated atomic pseudopotentials separately for atoms, Sb, Bi and Te by using the $5s^25p^3$, $6s^26p^3$ and $5s^25p^4$ configurations, respectively.

A. Structural Properties

Rhombohedral structure for Sb₂Te₃ and Bi₂Te₃, structures were considered in our calculation. The equilibrium lattice parameters have been computed minimizing the crystal's total energy calculated for the different values of lattice constant by means of Murnaghan's equation of states (eos) [23], and the results are shown in Table 1 along with the experimental and theoretical values. The lattice constants for Sb₂Te₃ and Bi₂Te₃ compounds are found to be $a = 4.256 \text{ \AA}$, $b = 30.397 \text{ \AA}$ and $a = 4.383 \text{ \AA}$, $b = 30.487 \text{ \AA}$, respectively. The lattice parameters obtained are in a good agreement with the experimental and theoretical values [24, 14]. In all our calculations, we have used the computed lattice constants.

TABLE 1. The calculated equilibrium lattice parameters (a , and c) together with the theoretical and experimental values for Sb₂Te₃ and Bi₂Te₃ in fractional coordinate.

Material	Reference	a (Å)	c (Å)
Sb ₂ Te ₃	Present (LDA-SIESTA)	4.256	30.397
	Theory (GGA-FLEUR) ^a	4.440	30.290
	Experimental ^b	4.250	30.350
Bi ₂ Te ₃	Present (LDA-SIESTA)	4.383	30.487
	Theory (GGA-FLUOR) ^a	4.530	30.630
	Experimental ^b	4.383	30.487

^aReference [14]

^bReference [28]

B. Elastic Properties

Here, to compute the elastic constants (C_{ij}), we have used the stress-strain method [25]. The present elastic constants for Sb_2Te_3 and Bi_2Te_3 are given in Table 2 along with the other theoretical and experimental results[15, 26,27].

TABLE 2. The calculated elastic constants (in GPa) for Sb_2Te_3 and Bi_2Te_3 .

Material	Reference	C_{11}	C_{33}	C_{44}	C_{66}	C_{12}	C_{13}
Sb_2Te_3	Present	83.2	99.7	44.6	31.0	21.2	46.1
Bi_2Te_3	Present	73.8	54.3	30.4	28.7	16.3	30.6
	Exp. ^a (280 K)	68.5	47.7	27.4	23.4	-	27.0
	Exp. ^a (0 K)	74.4	51.6	29.2	26.2	-	29.2
	Exp. ^b (77 K)	76.3	51.2	30.9	9.9	-	-
	Theory ^c (0 K)	69.0	54.8	28.8	26.7	-	21.6
	Theory ^c (300 K)	65.4	50.7	26.5	25.7	-	19.0

^aReference [30]

^bReference [31]

^cReference [15]

The elastic constants for Bi_2Te_3 are, generally, in accord with the theoretical and experimental results. The calculated C_{13} for Bi_2Te_3 is higher than the theoretical results. The C_{66} elastic constant at 77 K measured by Kullmann et al [27] for Bi_2Te_3 is significantly lower than the other results. These differences in the theoretical studies may originate from the different density-functional -based electronic structure methods. Unfortunately, there are no theoretical and experimental results for comparing with the present work for Sb_2Te_3 . The elastic constants C_{11} and C_{33} measure the a- and c- direction resistance to linear compression, respectively. The calculated C_{33} for Bi_2Te_3 is lower than the C_{11} , whereas the calculated C_{11} for Sb_2Te_3 is lower than the C_{33} . Thus, the c (a) axis for Bi_2Te_3 (Sb_2Te_3) are more compressible than the a (c) axis.

A problem arises when single crystal samples are not available, since it is then not possible to measure the individual elastic constants. Instead, the polycrystalline bulk modulus (B) and shear modulus (G) may be determined. There are two approximation methods to calculate the polycrystalline modulus, namely, the Voigt method and the Reuss method [28-30]. For specific cases of rhombohedral lattices, the Reuss shear modulus (G_R) and the Voigt shear modulus (G_V) are

$$G_V = \frac{1}{30} [M + 12C_{44} + 12C_{66}] \quad (1)$$

$$G_R = \frac{5}{2} (C^2 C_{44} C_{66}) / [3B_V C_{44} C_{66} + C^2 (C_{44} + C_{66})]$$

and the Reuss bulk modulus (B_R) and Voigt bulk modulus (B_V) are defined as

$$B_R = C^2 / M, \quad (2)$$

$$B_V = \frac{1}{9} [2(C_{11} + C_{12}) + 4C_{13} + C_{33}]$$

where, the abbreviations are $C^2 = C_{33}(C_{11} + C_{22}) - 2C_{13}^2$, $M = C_{11} + C_{12} + 2C_{33} - 4C_{13}$. Using energy considerations Hill [31] proved that the Voigt and Reuss equations represent upper and lower limits of the true polycrystalline constants, and recommended that a practical estimate of the bulk and shear moduli were the arithmetic means of the extremes. Hence, the elastic moduli of the polycrystalline material can be approximated by Hill's average and for shear moduli and bulk moduli it is

$$G = \frac{1}{2} (G_R + G_V) \text{ and } B = \frac{1}{2} (B_R + B_V) \quad (3)$$

The Young's modulus, E , and Poisson's ratio, ν , for an isotropic material are given by

$$E = \frac{9BG}{3B + G} \text{ and } \nu = \frac{3B - 2G}{2(3B + G)} \quad (4)$$

respectively [32,33]. Using the relations given above the calculated bulk modulus, shear modulus, Young's modulus, and Poisson's ratio for Sb_2Te_3 and Bi_2Te_3 are give Table 3.

It is known that isotropic shear modulus and bulk modulus are a measure of the hardness of a solid. The bulk modulus is a measure of resistance to volume change by an applied pressure, whereas the shear modulus is a measure of resistance to reversible deformations upon shear stress [34]. Therefore, isotropic shear modulus is better predictor of hardness than the bulk modulus. The isotropic shear modulus, a measurement of resistance to shape change, is more pertinent to hardness and the larger shear modulus is mainly due to its larger C_{44} . The calculated isotropic shear modulus and bulk modulus are 53.2, 32.5 GPa and 39.7, 24.8 GPa for Sb_2Te_3 and Bi_2Te_3 , respectively. The calculated bulk modulus for Bi_2Te_3 is a good agreement with experimental (0 K) [30] value. However, the bulk modulus is higher (about 7% and 11%) than the theoretical results. The calculated shear modulus for Sb_2Te_3 is higher than Bi_2Te_3 compound.

According to the criterion in refs. [34,35], a material is brittle (ductility) if the B/G ratio is less (high) than 1.75. The value of the B/G is less than 1.75 for Sb_2Te_3 and Bi_2Te_3 . Hence, these materials behave in a brittle manner.

TABLE 3. The calculated isotropic bulk modulus (B, in GPa), shear modulus (G, in GPa), Young's modulus (E, in GPa) and Poisson's ratio.

Material	Reference	B_H	G_H	ν	E
Sb_2Te_3	Present	53.2	32.5	0.246	80.9
Bi_2Te_3	Present	39.7	24.8	0.241	61.6
	Exp. ^a (280 K)	37.4	-	-	54.2
	Exp. ^a (0 K)	39.5	-	-	-
	Theory ^b (0 K)	34.4	-	-	52.5
	Theory ^b (300 K)	31.6	-	-	51.4

^aReference [30]

^bReference [15]

Young's modulus is defined as the ratio of stress and strain, and used to provide a measure of the stiffness of the solid. The material is stiffer if the value of Young's modulus is high. In this context, due to the higher value of Young's

modulus (80.9 GPa) Sb_2Te_3 compound is relatively stiffer than Bi_2Te_3 (61.6 GPa).

The value of the Poisson's ratio is indicative of the degree of directionality of the covalent bonds. The value of the Poisson's ratio is small ($\nu=0.1$) for covalent materials, whereas for ionic materials a typical value of ν is 0.25 [36]. The calculated Poisson's ratios are about 0.246, 0.241 for Sb_2Te_3 and Bi_2Te_3 , respectively. Therefore, the ionic contribution to inter atomic bonding for these compounds is dominant. The $\nu=0.25$ and 0.5 are the lower and upper limits, respectively, for central force solids [37]. Our ν values are close to the value of 0.25 indicating inter atomic forces are weightlessly central forces in Sb_2Te_3 and Bi_2Te_3 .

TABLE 4. The calculated shear anisotropic factors A_1 , A_2 , A_3 , and A_B , A_G

Material	Reference	A_1	A_2	A_B (%)	A_G (%)
Sb_2Te_3	Present	1.97	1.00	3.01	5.39
Bi_2Te_3	Present	1.81	1.00	0.10	5.71

The calculation of the elastic anisotropy is well established in the crystal physics. The elastic anisotropy arises from both shear anisotropy and the anisotropy of linear bulk modulus. For trigonal materials, the shear anisotropic factors for $\{100\}$ shear plane in $\langle 010 \rangle$ and $\langle 011 \rangle$ directions are $A_1 = 4C_{44}/(C_{11} + C_{33} - 2C_{13})$ and for $\{001\}$ shear plane in $\langle 010 \rangle$ and $\langle 011 \rangle$ directions are $A_2 = 2C_{66}/(C_{11} - C_{12})$ [38].

The calculated A_1 and A_2 for Sb_2Te_3 and Bi_2Te_3 are given in Table 4. A value of unity means that the crystal exhibits isotropic properties while values other than unity represent varying degrees of anisotropy. From Table 4, it can be seen that Sb_2Te_3 and Bi_2Te_3 exhibit low anisotropy. Another way of measuring the elastic anisotropy is given by the percentage of anisotropy in the compression (A_B) and shear (A_G) [32, 33, 39].

$$A_B = \frac{B_V - B_R}{B_V + B_R} \times 100 \quad \text{and} \quad A_G = \frac{G_V - G_R}{G_V + G_R} \times 100 \quad (5)$$

The percentage anisotropy values have been computed for Sb_2Te_3 and Bi_2Te_3 , and are shown in Table 4. For these compounds, it can be seen that the anisotropy in compression is small and the anisotropy in shear is high. Sb_2Te_3 compound exhibits relatively high bulk anisotropy between these compounds.

TABLE 5. The density, longitudinal, transverse, and average elastic wave velocities together with the Debye temperature.

Material	Reference	ρ (g/cm ³)	v_l (m/s)	v_t (m/s)	v_m (m/s)	θ_D (K)
Sb_2Te_3	Present	5.84	3840	2227	2472	232.3
Bi_2Te_3	Present	5.84	3040	1776	1969	181.3

The Debye temperature is known as an important fundamental parameter closely related to many physical properties such as specific heat and melting temperature. At

low temperatures the vibrational excitations arise solely from acoustic vibrations. Hence, at low temperatures the Debye temperature calculated from elastic constants is the same as that determined from specific heat measurements. We have calculated the sound velocities and the Debye temperature by using the common relation given in Ref. [40-42] for Sb_2Te_3 and Bi_2Te_3 .

C. Electronic Properties

The energy band structures calculated using LDA for Sb_2Te_3 and Bi_2Te_3 are shown in Fig. 1. As can be seen in Fig. 1, the Sb_2Te_3 and Bi_2Te_3 compounds have a direct band gap semiconductor with the values 0.093 eV and 0.099 eV, respectively. The top of the valance band and the bottom of the conduction band for both compounds positioned at the Γ point of BZ. In conclusion, our band gap values obtained are good agreement with theoretical values and the band gaps have same character with given in Ref. [6, 7]. Band structures of Sb_2Te_3 and Bi_2Te_3 single crystals are compared, band structures of these crystals are highly resemble one another. Thus, on formation of the band structures of Sb_2Te_3 and Bi_2Te_3 the 5s 5p orbitals of Te atoms are more dominant than 5s5p and 6s6p orbitals of Sb and Bi atoms.

Fig.1. Energy band structure, the total (DOS) and projected density of states for a) Sb_2Te_3 and b) Bi_2Te_3 .

The total and partial densities of states of Sb_2Te_3 and Bi_2Te_3 are illustrated in Fig. 1. As you can see, from this figure, the lowest valence bands occur between about -14 and -12 eV are dominated by Sb 5s and Bi 6s states while valence bands occur between about -12 and -10 eV are dominated by Te 5s states. The highest occupied valance bands are essentially dominated by Te 5p states. The 5p (6p) states of Sb (Bi) atoms are also contributing to the valance bands, but the values of densities of these states are so small compared to Te 5p states. The lowest unoccupied conduction bands just above Fermi energy level are dominated by Sb 5p and Bi 6p states.

III. CONCLUSION

In present work, we have made a detailed investigation of the structural, electronic, and mechanical of the Sb_2Te_3 and Bi_2Te_3 compounds using the density functional methods. The

results of the structural optimization implemented using the LDA are in good agreement with the experimental and theoretical results. The elastic constants obtained using the stress-strain method show that these compounds are mechanically stable. The related mechanical properties like shear modulus, Young's modulus, Poisson's ratio, Debye temperature, and shear anisotropic factors, sound velocities, and Debye temperature are calculated and discussed. The band gap calculated by using LDA for the Sb_2Te_3 and Bi_2Te_3 are direct band gap 0.093 eV and 0.099 eV, respectively.

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