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Effect of dilation on the electronic properties of Bi_2Te_3 compound: A first principal study

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***Abstract*— In this paper, we study the effect of dilation strain on electronic properties of Bi_2Te_3 compound, especially: band structure and density of state. Such studied are investigated by using in both first principles calculation and Boltzmann transport theory, based on DFT and calculated with GGA approximation. In evaluating a series of dilation strain values ranging from 0% to 3%, we notice a cancellation of band gap caused by overlapping of valance and conduction bands. Consequently we will have a growth of free charge with respect to the pure state (without expansion) and two region on the results of density of state which are: the core band and overlapping region.**

***Keywords*— Dilation, Bi_2Te_3, electronic properties, density functional theory, DOS**

I. INTRODUCTION

In recent times, much effort has been devoted to the study of thermoelectric materials [1],[2], for their importance in many applications, especially bismuth telluride compound (Bi_2Te_3). The electronic and thermoelectric properties of Bi_2Te_3 bulk [3]-[5], Bi_2Te_3 nanowires [6]-[8] and Nano-films [9]-[15], have been explored theoretically and experimentally. They have proved that to optimize the conversion efficiency of these materials types, they should have respectively the lowest and the strongest thermal and electrical conductivities as possible, to improve the factor of merit $ZT= T S^2\sigma/K$, Where S, σ, K represents Seebeck coefficient, electrical and thermal conductivity respectively. The electronic properties study can also give a vision on how to improve the performance of this material. Among the important approaches to strengthen the development efforts of thermoelectric devices, studied the effect of dilation on the optical properties of Bi_2Te_3 in the purpose to improve the conversion capacity at low temperature. At high temperature, there are materials present advantageous electronic and thermoelectric properties: for example, those based on magnesium Mg2X (X = Si, Sn, Ge, ...), whose the studies showed that are promising candidates in a range temperature between 300 and 800 K [16]-[18] and on the other as BiCuSeO [19], Zn_4Sb_3 [20], and recently they showed have an isostructural phase transition (IPT) under a hydrostatic pressure around 3 GPa [21]. We'll see their electronic behavior under expansion.

This work consists in evaluating the behavior of the band structure and also the carrier mobility and the density of state under expansion of Bi_2Te_3 using full potential linearized augmented plane wave FP-LAPW code implemented in the Wien2k package, with generalized gradient approximation (GGA). The Different theoretical and experimental studies have shown that strain can be used to control the band gap of TiO2, ZnO and MgO.

II. COMPUTATIONAL METHODS

In this part, we present the method that will be used through this paper. All the results presented are performed by using the full potential linearized augmented plane wave FP-LAPW code implemented in the Wien2k package [22]. It is noted that the FP-LAPW method divides the space into interstitial and non-overlapping muffin tin (MT) spheres. We use the Generalized Gradient Approximation (GGA) for the exchange correlation potential [23], [24], with the k-grid sampling of the Brillouin zone is 800 k-points.

For Bi_2Te_3 material, the Rayon Muffin Tin (RMT) used for Bi and Te atoms is 2.5. This compound crystallizes in a hexagonal-type structure at space-group 166_R-3m (see Fig. 1), with experimental lattice parameters a=b= 4,4 ° A ≠ c= 30.5 ° A[25].

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The atoms are ordered into positions: Bi (0.4001, 0.4001, 0.4001), Te1 (0, 0, 0), Te2 (0.2095, 0.2095, 0.2095). With their electronic configurations are: [Xe] 4f14 5d10 6s2 6p3, and [Kr] 4d10 5s2 5p4 for Bi and Te respectively. Under dilation, the parameters a and b depend on the percentage of expansion of interval [0%, 3%], for against the parameter along the z axis is calculated for each of the values.

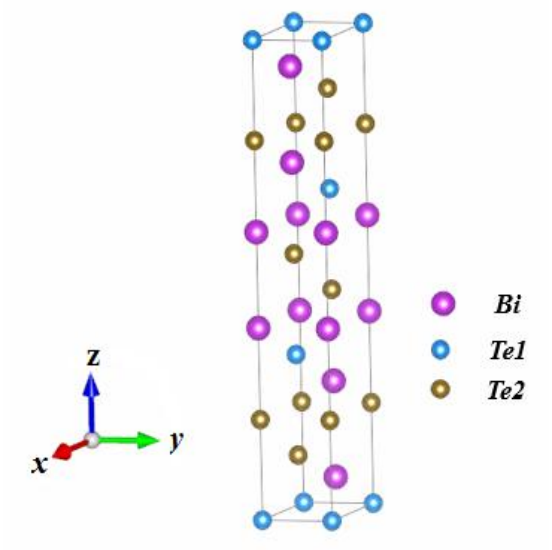

Fig. 1 Geometry representing the hexagonal unit cell of Bi_2Te_3

III. Results and Discussions

In the Bi_2Te_3, we study the effect of dilation strain on electronic properties. First we start by pure compound (without dilation). Then, we investigate the corresponding effect of this deformation we start by the geometry optimizations method in order to determine the equilibrium lattice parameters used later in the calculation. The obtained results of such parameters are a=b= 4,583 Å ≠c= 31,934 Å, α=β=90, and γ=120. These values are in good agreement with experimental results [25].

Taking these values, we calculate the band structure along high-symmetry Γ → M → K → Γ. The obtained results, as illustrated in Fig. 2a, show that the bottom of the conduction band and the top of the valence band are at the same point 'Γ', and other hand the value of gap energy is 0.3 eV. This indicates that this compound is a semiconductor with direct gap. This result correlates with previous work [26].

In order to inspect the origin of the charge transfer responsible of the obtained band gap, the total and partial density of states (DOS) are performed. The obtained results illustrated in Fig. 3a, show that we have three regions corresponding core, valence and conduction bands.

The core band (Cor.B) is located between -8 and -10.5 eV, in which the contribution of the s-orbitals of Te and Bi atoms is most. However the conduction band (CB) and the valence band (VB) is located between 0 and -4.2 eV and 0.6 and 5 eV respectively, in which the contribution of the p-orbitals of Te and Bi atoms is most.

For study the electronic properties of Bi_2Te_3 with dilation, we examined a series of dilation strain values ranging from 0% to 3%. The principle is to be applied a tensile in the XOY plane, which causes a variation of the parameter c which shrinks under tensile.

Taking this strain, the band structure, the total and partial density of states (DOS) are calculated. The obtained results, as illustrated in Fig. 2b and Fig. 3b. Under dilatation, there is an overlap of the two bands CB and VB (Metal), so this leaves only two regions: (Cor.B) and the overlap region on (Dos). The interatomic distance provided convincing explanation of the behavior. In fact the dilation is an increase in the interatomic distance, which leads to a fragility of bonds, consequently it facilitated their breaking and thereafter generates an increase of free loads and an increase in thermal and electrical conductivity.

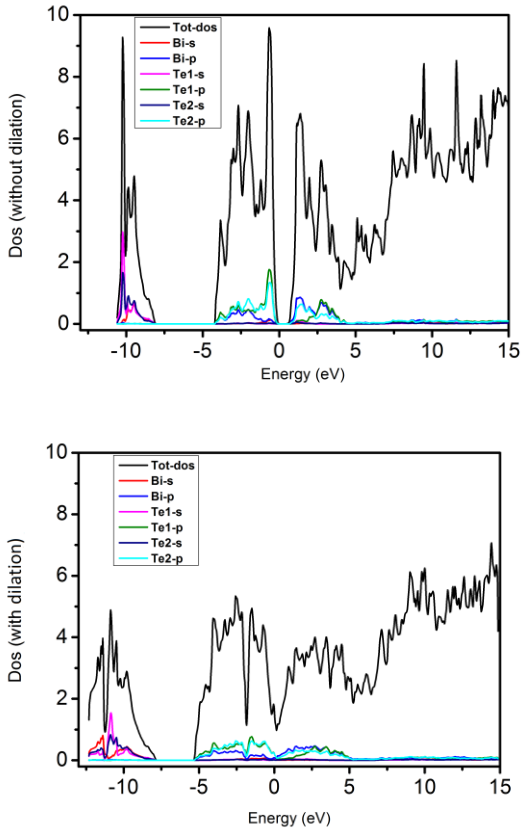

Fig. 2 Total and partial Dos for Bi_2Te_3 pure (a) and under dilation (b)

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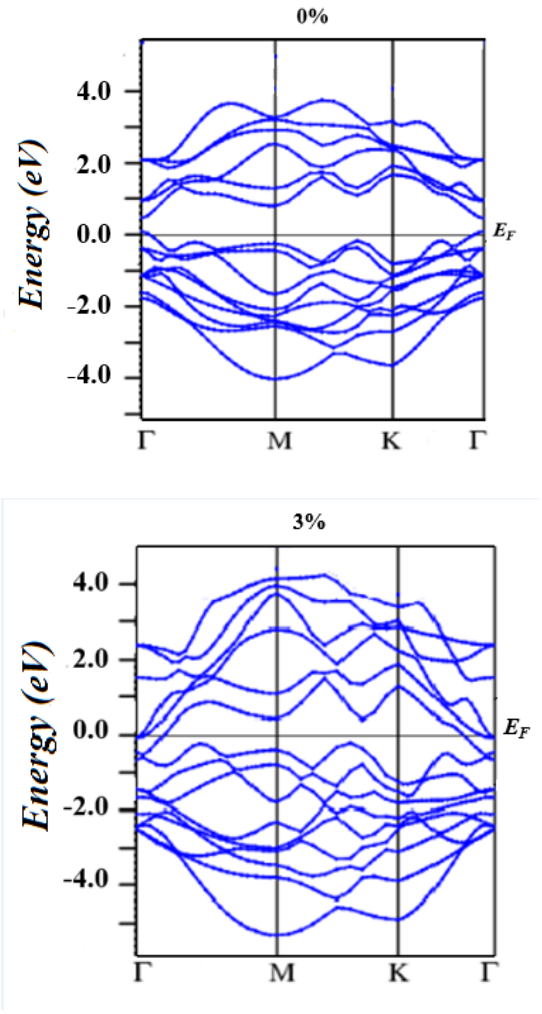

Fig. 2 Calculated band structure of Bi_2Te_3 pure (a) and under dilation (b)

IV. Conclusions

In conclusion, we have studied theoretically the effect of dilation strain on the Bi_2Te_3 electronic properties using first-principles calculations. Our density of state and structure band calculations showed, on one hand, that the valence band width expand depending on the strain value demonstrating the efficiency of an applied strain to provoke a motion of the energy band structure, on the other hand, it causes overlapping of two valence and conduction bands leave only two regions in the density of state.

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