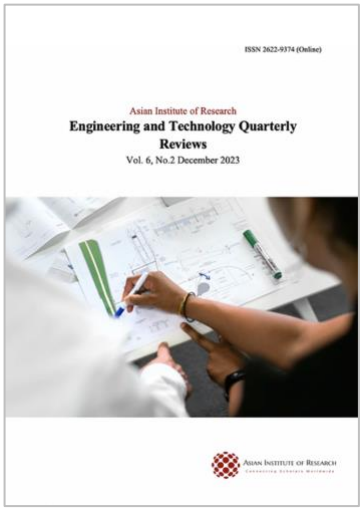

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Investigate the Bi2Se3 Crystal, which is a Three-Dimensional Topological Insulator

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Abstract
Topological insulators are materials that in bulk mode have band gap such as an ordinary insulator but can protect the conduction mode at the edge or surface, i.e. apart from a simple and insulated metal. These materials are insulator in their bulk modes but are metal at the surface. Topological insulators are developed in two and three dimensions. Recently, compounds of the Bi_2Se_3 have attracted a huge attention because of existence of a Dirac cone in their surface state, having a suitable bandgap (0.3 eV), and easy santhesis. In this research, we investigate the properties of this material using density functional theory. The main focus is on bulk calculations and surface properties. The band structure of this material is studied in bulk mode without any consideration of spin - orbit interaction. Then a surface of this material is considered and its band structure and density of states are studied. The results show that the surface of this material has a Dirac cone.

Keywords: Insulator, Density Function Theory, Bi2Se3, Topological Insulator, Band Structure, Dirac Cone

1. Introduction

Until the discovery of the quantum Hall effect in 1980 by Professor von Klitsenick (Moore, 2010), Different materials were classified based on symmetry failure. But with the discovery of the quantum Hall effect, it was seen that this new matter could not be classified on the basis of symmetry failure, because there are no more local order parameters here. A topological invariant is needed to describe the new phase.

Topological phases do not show any kind of failure of general symmetries and common local order parameters. These phases usually introduce insulation as a material that does not conduct electricity. In most insulators, the absence of electric current is described by the strip theory of solids. In recent years, a new type of insulation with a different topological strip structure with conventional insulation has been theoretically predicted. Accordingly, the new phase state is called topological insulation.

Topological insulations are theoretically predicted and experimentally observed in various systems including quantum wells (Bernevig, Hughes, & Zhang, 2006; König et al., 2008) HgTe, alloys such as Bi2Sb3 (Gehring et al., 2013; M. Zahid Hasan & Charles L. Kane, 2010) and Bi2Te3 (M. Z. Hasan & C. L. Kane, 2010) and crystals of Bi2Se3 (Gehring et al., 2013; M. Z. Hasan & C. L. Kane, 2010) Is. In topological insulations, if a perpendicular exchange field enters its surface, it can eliminate surface states and the conductive surface of the topological insulator behaves like an insulator. If the exchange magnetic field enters in the direction of the plate, it has no effect on the surface states. Topological insulations are divided into two parts: two-dimensional insulations and three-dimensional insulations and have been studied.

The most basic state of a material is the state of insulation, and insulation is a material that has an energy gap that separates full and empty strips. The simplest insulator is an atomic insulator, in which electrons are attached to atoms in closed shells.

Due to the quantum hall, a strong magnetic field is applied to the two-dimensional electron gas system at very low temperatures. Under the conditions, it is observed that there is current inside the surface of the insulation system and only at the edges, and the changes in the resistance of the hall in terms of field are no longer linear, but change stepwise(M. Z. Hasan & C. L. Kane, 2010).

$$\sigma_{xy} = \frac{Ne^2}{h} \qquad (1)$$

In this interface N is an integer (N = 1,2,3…). In quantum effects, the inverse symmetry of time is broken due to the presence of an external magnetic field.

Due to quantum spin, the direction of motion of electrons depends on its spin direction, and electrons with different spins move in two opposite directions. Having the inverse symmetry of time prevents these edge currents from scattering in the presence of impurities (non-magnetic). The presence of such spin currents without scattering and in the absence of an external magnetic field is useful for use in Tronic Spins. The effect of quantum hall spin was theoretically predicted in 2006 by Bernevig , Hughes, and Zheng in the mercury telluride quantum well (M. Z. Hasan & C. L. Kane, 2010) and was experimentally observed in 2007 by Koenig et al. (M. Z. Hasan & C. L. Kane, 2010).

Topology is actually a mathematical concept used in mathematics for general classification of shapes. In fact, shapes can be transformed by dragging and turning into another shape. Of course, without tearing, these shapes are topologically equivalent, but may be different in appearance. It must be borne in mind that the mathematical concept of the Gauss-Bonne theorema more, if we take the integral from the curvature of Barry in the Brillouin region, the results will always be discrete values, which are called Chern number (Kane, 2008; Liu et al., 2011). The topological classification in terms of the Chern number, also called the TKNN invalid in physics, is for insulators in which the symmetry of time reversal is broken. In insulations in which the inverse symmetry of time is maintained (insulations are two-dimensional or the same effect of quantum hall spin), the Chern number is zero (M. Zahid Hasan & Charles L. Kane, 2010). Therefore, to classify them, another topological invalid is needed, which is called Z2 invalid (M. Zahid Hasan & Charles L. Kane, 2010). Invalidity of Z2 takes two values of zero and one. For example, it becomes zero for a vacuum and equal to one for the quantum Hall effect. Only one Z2 invariant is required to classify two-dimensional topological insulation, and four Z2 invariant is required to classify three-dimensional topological insulation (Fu, Kane, & Mele, 2007).

Three-dimensional topological insulation (which is insulated in volume but has conductive surfaces) was also theoretically predicted in 2007 by Liang Fu and Qin (M. Z. Hasan & C. L. Kane, 2010) and was observed experimentally in 2008 by Hsieh et al (M. Z. Hasan & C. L. Kane, 2010; Lin et al., 2010). In 2009, Hsieh et al. Experimentally observed a three-dimensional sample of topological insulation (Bi2Se3), which has two special advantages over previous samples (M. Zahid Hasan & Charles L. Kane, 2010; Maciejko et al., 2009). First, it has a larger energy gap (about 0.3ev) than previous models such as the Bi2Sb3, which gives it a topological insulation at room temperature. Second, its surface states have only one Dirac point in the gap, which is the simplest possible situation. Topological insulators have special properties that can be useful for applications from spintronics to quantum computing.

2. Brief introduction of topological insulators

As mentioned earlier, topological insulators are materials that are insulating in volume but have conductive properties along their boundaries. In fact, along the mazes, there are edge states that are without gaps, these metal edge alignments are formed by the specific topology of these materials.

Topology is essentially a branch of mathematics in which mathematicians divide geometric objects into different topological categories (Figure1). The topological branches of each geometric shape assign a topological number (constant) called the topological constant. In fact, the difference between topological insulation and conventional insulation is in their topological constant. Heavy elements as well as semiconductors with small energy gaps are better candidates for making topological insulations. Theoretical and experimental predictions of topological states in two and three dimensions, has made one of the most important and growing topics in the physics of dense matter today. Apart from being an important tool for basic concepts, topological insulators are also used in chemicals, and they also provide new ways to build and produce new devices, which are widely used in the spintronics industry and quantum computing.

In addition to experimental advances, there is a need for atomic modeling of these materials, which allows for quantitative predictions and comparisons with experiments. Significant advances have been made in the initial methods for calculating the electrical and magnetic properties of TI (Pertsova & Canali, 2014).

Figure 1: Example of two objects that are topologically different.

3. A review of the crystal composition of Bi2Se3

Because the research element of this dissertation is the composition of Bi_2Se_3 crystal, first, the Bise crystal is briefly introduced. The Bi_2Se_3 family of compounds a rhombohedral crystal structure with space group D_{3d}^5 $R\bar{3}m$, we take Bi_2Se_3 as an example in the following. As shown in figure 2(a), the system has a layered structure with five atomic layers as a basic unit (cell), named a quintuple layer (QL). The inter-layer bonding within the QLs is strong because of the dominant covalent character, but the bonding between the QLs is much weaker due to the van der Walls-type interaction. The binary (with twofold rotation symmetry), bisectrix (appearing in the reflection plane) and trigonal (with threefold rotation symmetry) axes are taken as the x, y and z axes, respectively, and the primitive translation vectors $t_{1,2,3}$ shown in figure 2 are

$$t_1 = \left(-\frac{a}{2}.-\frac{\sqrt{3}a}{6}.\frac{c}{3}\right).t_2 = \left(\frac{a}{2}.-\frac{\sqrt{3}a}{6}.\frac{c}{3}\right)\text{، }t_3 = \left(0.\frac{\sqrt{3}a}{3}.\frac{c}{3}\right) \qquad (2)$$

Here, a and c are lattice constants in the hexagonal cell. The corresponding reciprocal vectors $s_{1,\,2,\,3}$ defined by $S_i.t_j = 2\pi\delta_{ij}$ are given as(Zhang, Yu, Zhang, Dai, & Fang, 2010)

$$s_1 = \left(-1\text{،}-\frac{\sqrt{3}}{3}\text{،}b\right)h\text{،}\ s_2 = \left(1\text{،}-\frac{\sqrt{3}}{3}\text{،}b\right)h\text{،}\ s_3 = \left(\frac{0.2\sqrt{3}}{3}.b\right)h \qquad (3)$$

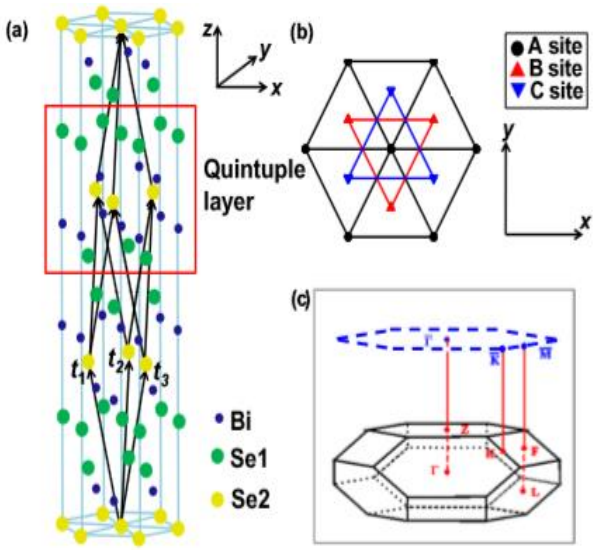

Figure 2. Crystal structure of the Bi_2Se_3 family of compounds. (a) The hexagonal supercell containing 15 atomic layers and primitive translation vectors $\mathbf{t}_{1,2,3}$. (b) The top view of a QL in the triangle lattice. Three sets of different sites, labeled as A, B and C sub lattices, respectively, are presented. Owing to the D_{3d}^5 symmetry, the stacking of atomic layers along the z-direction is the order of …-C(se1)-A(se1)-B(Bi)-C(se2)-A(Bi)-B(Se1)-C(se1)…(c) The first BZ. Four nonequivalent TRIM points $\Gamma(0,0,0)$, $L(\pi,0,0)$, $F(\pi,\pi,0)$, and $Z(\pi,\pi,\pi)$ are denoted in the 3D BZ. The corresponding surface 2D BZ is represented by the dashed blue hexagon, and $\bar{\Gamma}$, $\bar{M}$ and $\bar{K}$ are the corresponding TRIM special K points in the surface BZ(Zhang et al., 2010).

With

$$b = \frac{a}{c} \quad , \quad h = \frac{2\pi}{a} \tag{4}$$

As shown in figure 2(a), we take Se2 to be at the origin (0,0,0), then two Bi sites are at $(\pm\mu \pm \mu \pm \mu)$, and two Se1 are at $(\pm v \pm v \pm v)$, defined in the unit of primitive translation vectors. All the experimental lattice parameters and internal parameters μ and v are listed in table 1. Figure 2(c) shows the 3D first Brillouin zome (BZ) and the 2D surface BZ of Bi_2Se_3. $\Gamma(0,0,0)$, $L(\pi,0,0)$, $F(\pi,\pi,0)$, and $Z(\pi,\pi,\pi)$ are four time-reversal invariant momentum (TRIM) points in 3D BZ. $\Gamma(0,0,0)$ and $Z(\pi,\pi,\pi)$ are projected as $\bar{\Gamma}$, and $L(\pi,0,0)$ and $F(\pi,\pi,0)$, are projected as $\bar{M}$ in the surface BZ. For the choice of our cell, Bi_2Se_3 has the inversion symmetry with inversion center at Se_2. The space group $R\bar{3}m$ can be constructed from three symmetry generators: I (inversion), C_{3Z} (threefold rotation around z) and σ_x (mirror plane with its normal along x)(Hixson & Fritz, 1992; Zhang et al., 2010).

4. Calculation of the band structure of Bi2Se3 crystal compound

Bi_2Se_3 crystal is a strong three-dimensional topological insulator. We want to calculate its band structure. In calculating the strip structure, a five-layer crystal is used, each layer containing three atoms, which is a total of 15 atoms. It should be noted, however, that the Bi_2Se_3 crystal in this calculation contains five atoms in a single cell (of which 2 atoms belong to bismuth and 3 atoms to selenium). The crystal structure of Bi_2Se_3 was fabricated using ATK software. The strip structure of Bi_2Se_3 with and without spin-circuit interaction (SOC) was also calculated. In the calculation by approximation, the generalized slope gradient or gga (taking into account the spin-orbit) shown by Figure (3) forms a direct gap of 0.1255 eV at the gamma point. spin-orbit pairing in sogga calculations has a significant effect on the band structure, which expands the direct band gap at the gamma point and forms an indirect gap such that a band gap in the sogga calculation (excluding spin-orbit) It is 0.3202 eV, as shown in Figure (4). Bi_2Se_3 crystal is still semiconductor.

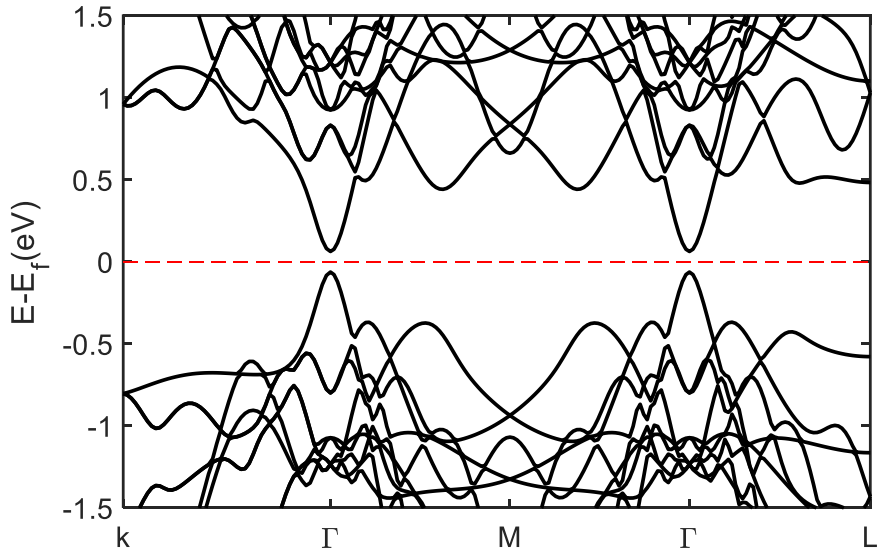

Figure 3: Shows the bulk band structure of Bi2Se3 crystal with gga calculation.

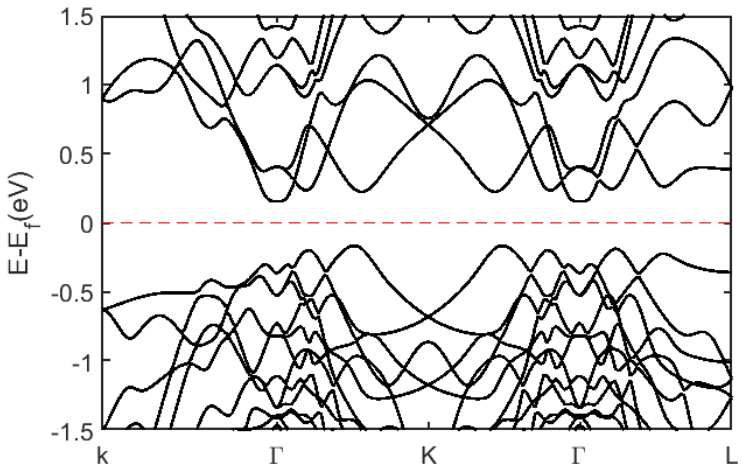

Figure 4: Shows the bulk band structure of Bi2Se3 calculated by sogga.

5. Calculation of the band structure of the two-dimensional cut sheet (slab) of the Bi2Se3 crystal

The calculation of the shear bond structure of the Bi_2Se_3 crystal is shown in Figure (5). In this case, only the calculation is done with sogga, which shows significant changes in the crystal structure. A small, direct gap (0.0077 eV) is formed at the gamma point, and the Dirac cone is still clearly visible inside the band gap. In fact, we are witnessing a topological behavior. The transition from the bulk to a cut sheet has led to the appearance of the Dirac cone and the closure of the gap.

It is further noted that the electronic structure of the surface states close to the Fermi surface resembles a Dirac cone, where the electron momentum depends linearly on the energy. Since surface states are the only states present within the bulk energy gap, we should expect the electron density of states close to Fermi energy (E_f) to be linear. Here we calculate the electron density, in the calculated diagram of the electron density of the Dirac cone above the Fermi energy level. The electron densities of bismuth and selenium were calculated separately, the result showing that the p orbital has the highest share in both elements and the s orbital has the lowest share in both elements. As can be seen in the Bi2Se3 crystal, the share of selenium is higher than that of bismuth, which is shown by Figures (6, 7 and 8).

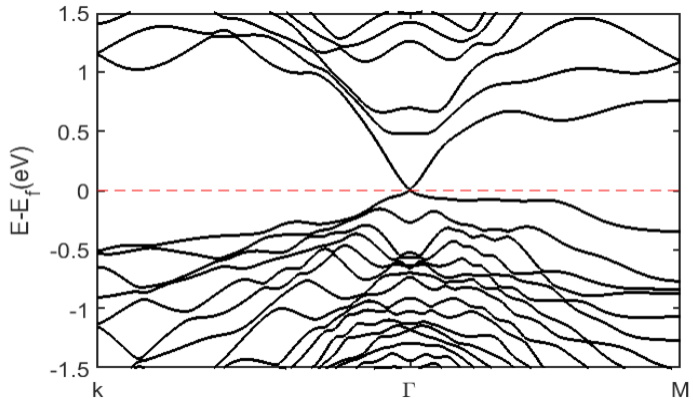

Figure 5: Shows the band structure of Bi2Se3 cut sheet by sogga calculation.

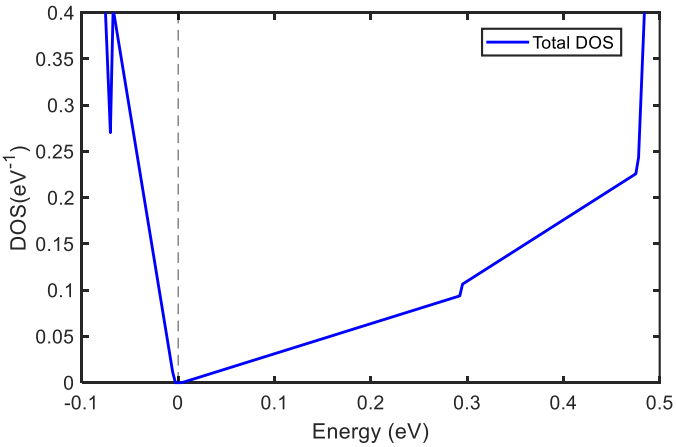

Figure 6: Shows the electron density diagram of the cut sheet of Bi2Se3.

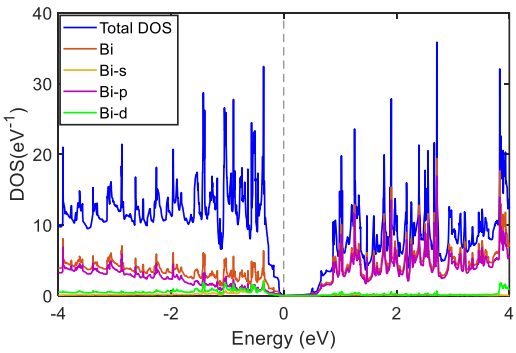

Figure 7: Shows the comparison of the total electron density with the electron density of bismuth crystal Bi2Se3.

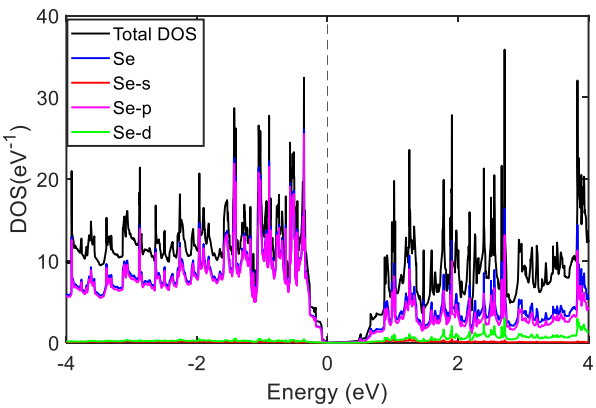

Figure 8: Shows the comparison of the total electron density with the electron density of Bi2Se3 crystal selenium.

6. Apply strain to Bi_2Se_3 crystal

Bi_2Se_3 crystal is chemically stable, showing a strong topological phase for easy synthesis. Theoretical and experimental studies that have been done on it, introduce it as a prototype of topological insulation and is a natural choice for initial research. There is also interest in the effect of mechanical strain on topological effects. There is also interest in the effect of mechanical strain on topological effects. Therefore, for the Bi_2Se_3 block mode, the effect of arbitrary pressures of 2% and - 2% on the gap at the gamma point and with the bond structure with spin-orbit interaction has been calculated. It was observed that the application of 2% strain (tensile strain) reduces the energy gap and reaches 0.0095 eV and is straight. From the obtained electron density of the mentioned structure, it can be seen that the Dirac cone is below the Fermi energy level, indicating the metallization of the Bi_2Se_3 crystal.

By applying a 2% strain, the band gap is reduced to about (0.0083 eV) and is straight. It has a Dirac cone structure, in which the gap and the Dirac cone both form above the Fermi energy level at the gamma point, thus increasing the semiconductor properties of the Bi_2Se_3 crystal. Also, the electron density of the relevant structure has been calculated, which indicates the Dirac cone on the Fermi energy surface and indicates that the Bi_2Se_3 crystal is semiconductor. All results are shown by Figures (11, 12, 13 and 14) below.

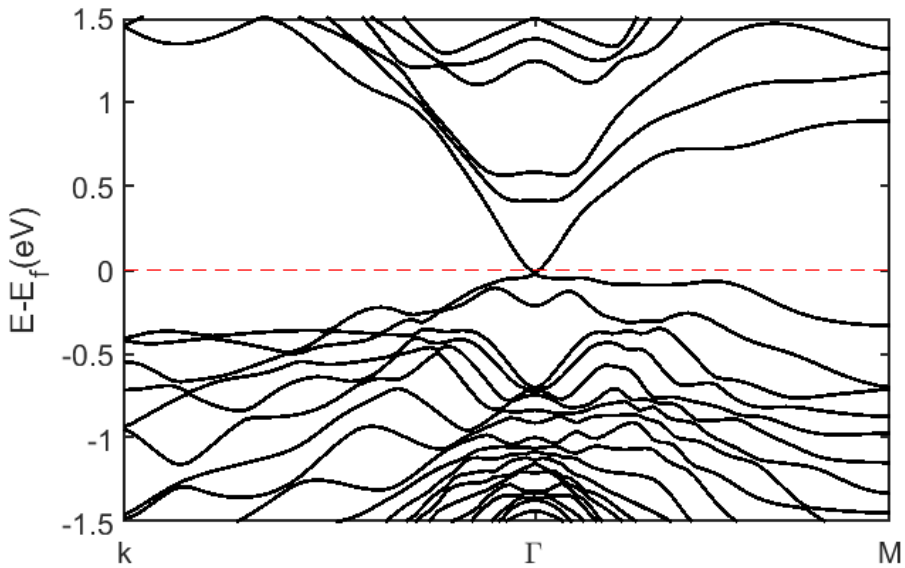

Figure 9: Shows the energy band structure diagram of applied 2% Bi2Se3 strain.

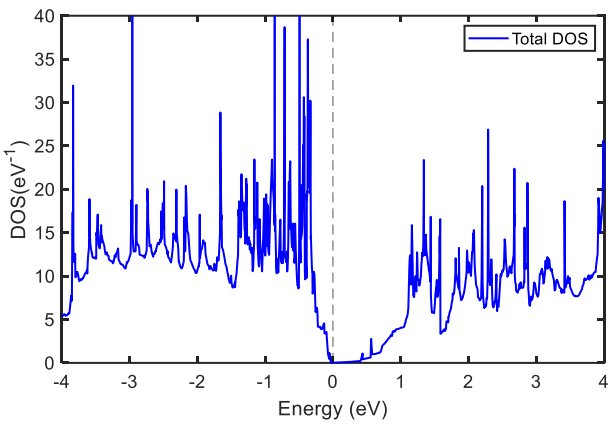

Figure 10: Shows the electron density diagram of 2% strain applied to the Bi2Se3 crystal

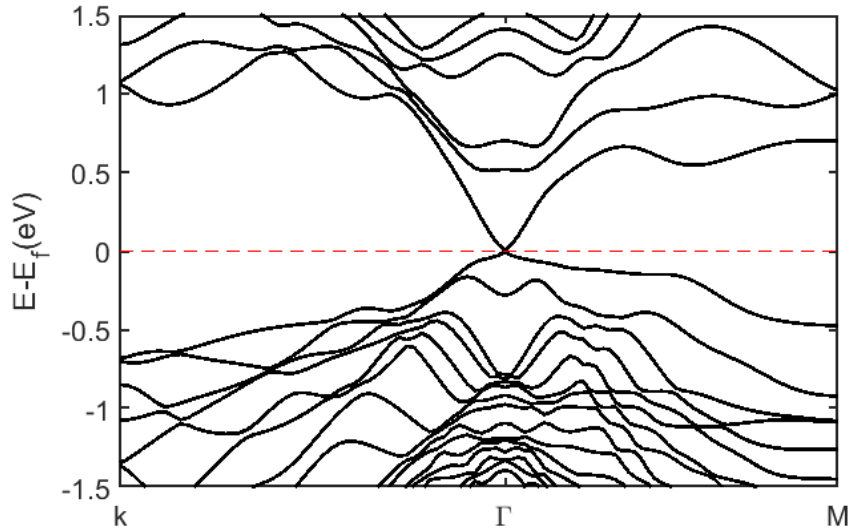

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Figure 11: Shows the energy band structure diagram of -2% applied strain on the Bi2Se3 crystal.

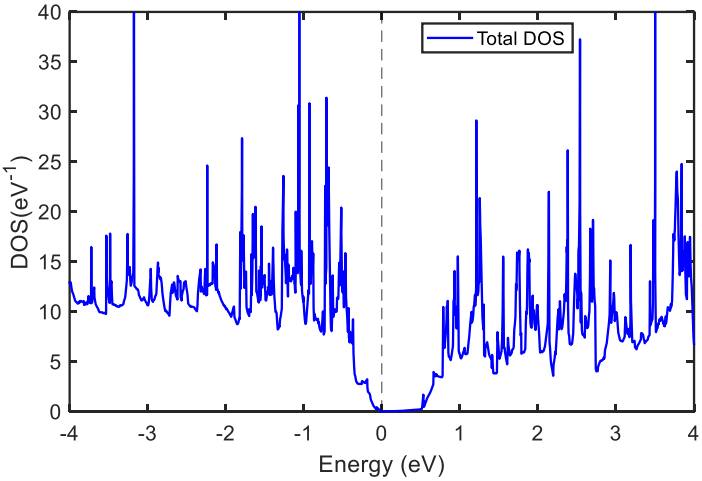

Figure 12: Shows the electron density diagram of -2% strain applied to the Bi2Se3 crystal.

7. Conclusion

In this research, first an attempt was made to form the crystal structure of Bi2Se3, and the band structure, total electron density, electron density of each element of bismuth and selenium were calculated separately and compared. In calculating the band structure before cutting, a bigger gap was obtained.

After cutting the gap, the energy of the Bi2Se3 bond structure decreased and its semiconductor properties increased. For larger gap cuts, the energy will decrease more and the crystal will become semi-conducting. In addition, 2% and -2% strain were also applied to the Bi2Se3 crystal. After calculating its band structure and electron density, it was observed that tensile strain cause a further reduction of the energy gap. From the observations of the obtained results, it can be said that the metallic properties of the Bi2Se3 crystal have increased and can go towards metallization.

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