Topological Insulation And Bi2Se3 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 Bi2Se3 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 synthesis. 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 - Density Function Theory; Bi2Se3 ;Topological Insulator, Band Structure, Dirac Cone, Metal

I. Introduction

Until the discovery of the quantum Hall effect in 1980 by Professor von Klitsenick[1], 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[2, 3] HgTe, alloys such as Bi2Sb3[4, 5] and Bi2Te3[6] and crystals of Bi2Se3[5, 6] 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[6].

\[ \sigma_{xy} = \frac{N e^2}{\hbar} \]  

(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[6] and was experimentally observed in 2007 by Koenig et al[6].

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
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[7, 8]. 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 insulators in which the inverse symmetry of time is maintained (insulators are two-dimensional or the same effect of quantum hall spin), the Chern number is zero[4]. Therefore, to classify them, another topological invalid is needed, which is called Z2 invalid[4]. 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[9].

Three-dimensional topological insulation (which is insulated in volume but has conductive surfaces) was also theoretically predicted in 2007 by Liang Fu and Qin[6] and was observed experimentally in 2008 by Hsieh et al[6, 10]. In 2009, Hsieh et al. Experimentally observed a three-dimensional sample of topological insulation (Bi2Se3), which has two special advantages over previous samples[4, 11]. 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.

A. Insulators

The most basic state of the material is the state of isolation; The simplest insulator is an atomic insulator, to which electrons are attached to its atoms in closed shells. Such a substance is electrically neutral because it uses electrical energy to move an electron. Because we know that a strong interaction between atoms creates a covalent bond. One of the recent successes of quantum physics was the development of the strip theory of solids, which provided the description of the electronic structure of such states. This theory is exploited by using the crystal transition symmetry to classify electronic states in terms of the K-momentum of the crystal itself, defined in a period Brillouin region. |m⟩ The Bloch state in a single crystal cell belongs to the Hamiltonian H (k) Bloch. Energy bands are defined by specific numbers Em (k) that make up the entire band structure. In insulation, an energy gap separates the capacitance strip states (full strip) from the conductive strip states (empty strip). Although the gap in an atomic insulator, such as solid argon, is much larger than that of a semiconductor, they both belong to the same phase. It is possible to reach another by correcting and manipulating Hamilton continuously without closing the tape gap. Such a process defines a topological equivalence between different insulators. In fact, all conventional insulators are topologically equivalent to vacuum, which according to Dirac’s quantum theory of relativity has energy gaps (for generating pairs), conductive bands (electrons), and capacitance bands (positrons)[4].

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[12].

Figure (1) is an example of a mathematical topology figure
B. Crystal composition Bi₂Se₃

Because the research element of this dissertation is the composition of Bi₂Se₃ crystal, first, the Bise crystal is briefly introduced.

The Bi₂Se₃ family of compounds a rhombohedral crystal structure with space group $D^{3}_{d}$, $R3m$, we take Bi₂Se₃ 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.

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 $(\pm \nu \pm \nu \pm \nu)$, defined in the unit of primitive translation vectors. All the experimental lattice parameters and internal parameters $\mu$ and $\nu$ are listed in table 1. Figure 2(c) shows the 3D first Brillouin zone (BZ) and the 2D surface BZ of Bi₂Se₃. $\Gamma(0\cdot0\cdot0)$, $L(\pi\cdot0\cdot0)$, $F(\pi\cdot\pi\cdot0)$, and $Z(\pi\cdot\pi\cdot\pi)$ are four time-reversal invariant momentum (TRIM) points in 3D BZ. $\Gamma(0\cdot0\cdot0)$ and $Z(\pi\cdot\pi\cdot\pi)$ are projected as $\bar{\Gamma}$, and $L(\pi\cdot0\cdot0)$ and $F(\pi\cdot\pi\cdot0)$, are projected as $\bar{M}$ in the surface BZ. For the choice of our cell,

\begin{equation}
\begin{align*}
 b & = \frac{a}{c} \quad \text{and} \quad h = \frac{2\pi}{a} \\
\end{align*}
\end{equation}
Bi$_2$Se$_3$ has the inversion symmetry with inversion center at Se$_2$. The space group $R\overline{3}m$ can be constructed from three symmetry generators: I (inversion), $C_{3z}$ (threefold rotation around $z$) and $\sigma_x$ (mirror plane with its normal along $x$)\[13, 14\].

Table (1) shows the laboratory network parameters and internal parameters of Bi$_2$Se$_3$ family compounds\[13\].

<table>
<thead>
<tr>
<th></th>
<th>Sb$_2$Te$_3$</th>
<th>Bi$_2$Te$_3$</th>
<th>Bi$_2$Se$_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice constant $a$ (Å)</td>
<td>4.250</td>
<td>4.383</td>
<td>4.138</td>
</tr>
<tr>
<td></td>
<td>$c$ (Å)</td>
<td>30.35</td>
<td>30.487</td>
</tr>
<tr>
<td>Inner coordinates $\mu$</td>
<td>0.400</td>
<td>0.400</td>
<td>0.399</td>
</tr>
<tr>
<td></td>
<td>$\nu$</td>
<td>0.211</td>
<td>0.212</td>
</tr>
</tbody>
</table>

II. Calculation of insulation band structure of Bi$_2$Se$_3$ topology

Bi$_2$Se$_3$ 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$_2$Se$_3$ 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$_2$Se$_3$ was fabricated using ATK software. The strip structure of Bi$_2$Se$_3$ 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$_2$Se$_3$ crystal is still semiconductor.

Figure (3) shows the calculation and plotting of the Bi$_2$Se$_3$ band structure with gga

Figure (4) shows the calculation and plotting of the Bi$_2$Se$_3$ bond structure with sogga.
A. Calculation of two-dimensional cut sheet strip structure (slab) Bi$_2$Se$_3$

The calculation of the shear bond structure of the Bi$_2$Se$_3$ 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 Bi$_2$Se$_3$ crystal, the share of selenium is higher than that of bismuth, which is shown by Figures (6, 7 and 8).

![Figure (5) shows the calculation and drawing of the band structure of a cut sheet of Bi$_2$Se$_3$ with sogga](image)

![Figure (6) shows the calculation of the electron density of the cut sheet of Bi$_2$Se$_3$](image)
Figure (7) shows a comparison of the total electron density with the electron density of Bi$_2$Se$_3$ crystal bismuth.

Figure (8) shows a diagram comparing the total electron density with the electron density of Bi$_2$Se$_3$ crystalline selenium.

**B. Depth of penetration of surface states**

Expansion of surface modes, in other words the depth of spatial penetration in the bulk, is an essential value for potential applications of surface modes. One of the main features of protected surface modes close to Dirac point is that they are highly substituted to the surface area. We use a sheet consisting of 15 QL, direct connection between the two levels should be avoided, i.e., the electronic states of the upper and lower surfaces of the sheet should not be connected. The bond structure calculated from the 15-QL cut-off sheet of Bi$_2$Se$_3$ along the line G → K and G → M is shown in Figure (9). In addition, the observed flatness of the surface modes in the calculation of the band structure at any particular point K consists of modes with opposite spins and are placed on opposite sides of the cut plate. By moving away from the Dirac point, the penetration depth increases, and suddenly for the larger k-points, where the surface state almost merges with the large state, the wave function becomes a wide state. Then both Bloch states are cut on the C axis of the unit cell of the page and the scale and direction of the spin vectors of the other line are plotted as a function of the C coordinates.

The positions are located on both sides of the cut page and their spin directions are opposite to each other. The orange and purple dots in Figure (9) indicate the position of the Se and Bi atoms. The two modes are clearly on opposite sides of the cut plate (red curve) and there is very little overlap in the middle. The polar angle is 270 degrees for both modes (blue curve), but the surface angle for the 144 band is 120 degrees and for the 145 band (green curve) is 300, which indicates a 180-degree rotation, meaning that the spin direction is on both sides of the image. Therefore, the two spin modes point in the opposite direction. Finally, it can be concluded that the surface modes are highly alternated to the surface area and the penetration depth is about 2 or 3 QL.
Figure (9) shows the penetration depth of Bi$_2$Se$_3$.

C. Bi$_2$Se$_3$ Fermi level calculation

The study of the Fermi surface of the cut sheet of Bi$_2$Se$_3$ crystal in the vicinity of Dirac cone is very significant. This is easily located by sampling the band structure on a dense spherical network at the center of the gamma. The result scheme is shown below by Figure (10). As expected for the Dirac cone, the Fermi surface is a circle near the end (red dot), but turns into a hexagon with larger energies. Here, the line corresponding to the energy $E = 0.15$ eV is extracted and the Bloch state for each point ($K_x$ and $k_y$) around this distance is calculated. At each point, an arrow indicates the direction of the spin on the surface. The spin is rotated at an angle of $2\pi$ in such a way that it rotates around the Dirac point. The reason for this is simple, because the symmetry of time reversal requires that the states in $k$ and $-k$ have opposite spins. However, the Dirac cone is not for surface states where the origin of a surface is a spin. However, Dirac cones do not degenerate spin for surface modes that originate from a surface. Therefore, the spin must rotate with $k$, as it is around the Fermi surface. Accordingly, the calculation of the $\pi$-phase separation closed by the Fermi surface state is one of the methods for detecting TI topological insulation, each of which forms an orbital spin that carries the $\pi$-phase phase. And shows the topological properties of Bi$_2$Se$_3$.

Figure (10) shows the Fermi surface of Bi$_2$Se$_3$.

D. Apply strain to Bi$_2$Se$_3$ crystal

Bi$_2$Se$_3$ 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. Therefore, for the Bi$_2$Se$_3$ 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$_2$Se$_3$ 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$_2$Se$_3$ 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$_2$Se$_3$ crystal is semiconductor. All results are shown by Figures (11, 12, 13 and 14) below.

Figure (11) shows the calculation and plotting of the applied energy band structure of 2% above Bi$_2$Se$_3$.

Figure (12) shows the electron density of a 2% Bi$_2$Se$_3$ biaxial tensile strain.
Figure (13) shows the calculation and plotting of the energy band structure of the applied strain -2% above Bi$_2$Se$_3$.

Figure (14) shows the electron density of a compression strain of -2% for Bi$_2$Se$_3$.

III. Conclusion

In this study, we investigated Bi$_2$Se$_3$, which is a three-dimensional topology insulator, using the DFT method. The crystalline compounds of the Bi$_2$Se$_3$ family have a hexagonal crystal structure with a space group R3m and a symmetry of $D_{3d}^5$. The system has a layered structure with five atomic layers in a single cell, called a five-layer layer. Interlayer bonding is predominant in QLs due to the coulomb bonding property, but bonding between QLs is very weak due to a Wonder-Wall interaction. In this combination, a and c are the lattice vectors in a hexagonal cell (a = 4.138 and C = 28.64). ($\mu = 0.399$ and $\nu = 0.206$) are the constants of the mentioned crystal lattice. Bi$_2$Se$_3$ has an energy gap of about 0.3 eV and is also chemically stable and easy to synthesize, which is of greater importance for research due to its small gap.

First, an attempt was made to form a Bi$_2$Se$_3$ crystal structure, in which the bond structure, penetration depth and Fermi surface were calculated. A larger gap was obtained in calculating the band structure before cutting. After cutting the gap, the energy of the Bi$_2$Se$_3$ bond structure decreased and its semiconductor properties increased. For large gap gaps, more energy is reduced and the crystal will become semiconductor. In addition, strain was applied to the Bi$_2$Se$_3$ crystal, which further reduced the energy gap. From the observed results, it can be said that the metallic properties of Bi$_2$Se$_3$ crystal increase and lead to metallization.
IV. References