First-principles study of electric-field-induced topological phase transition in one-bilayer Bi(111)

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Using first-principles calculations, we determined the topological phase transition induced by electric fields in one-bilayer Bi(111). The bandgap is decreased from 0.32 to 0 eV when the applied electric field reaches 2.1 V/Å. Further increasing the applied electric field opens the bandgap, which reaches 0.34 eV at 4.0 V/Å. We computed the Z2 invariant that characterizes topological insulator phases. As results, one-bilayer Bi(111) showed a topological phase transition induced by the electric field, from the topological insulator phase to the trivial insulator phase through a Dirac semimetal. This topological phase transition could be applied to novel devices. © 2018 The Japan Society of Applied Physics

Topological insulators have attracted considerable research attention for their possible applicability to novel devices.1) A topological insulator is a nontrivial insulator phase caused by time-reversal symmetry and spin–orbit interactions. The phase has stable metallic edge states protected by time-reversal symmetry; therefore, the metallic edge states are robust against non-magnetic impurities. In addition, the edge states have dissipation-free spin currents. Because of the lack of back-scattering in the edge spin current, the topological insulator could be applied to materials of novel devices.

In order to achieve on/off electrical switching of the edge spin current, i.e., to create a trivial-to-topological switching device, the topological phase transition between the topological insulator phase and trivial-insulator phase must be controlled, which requires closing the bandgap. Topological phase transitions induced by electric fields have been predicted for the two-dimensional material of phosphorene.2) This material can be applied to a novel transistor by using the topological phase transitions from the trivial insulator into the topological insulator, where the 0.1 eV bandgap of the four-layer phosphorene closes for an electric field E = 0.3 V/Å.2)

It is worth investigating the materials in topological-to-trivial electrical switching devices. One-bilayer Bi(111) is one such candidate material and it could be formed on Si(111) experimentally.3) In addition, it has been reported theoretically4,5) and experimentally6,7) as a topological insulator, where the 0.1 eV bandgap of the four-layer phosphorene closes for an electric field E = 0.3 V/Å.2)

In this study, we investigate the effect of an electric field on a one-bilayer Bi(111) film, where the electric field is applied up to 4.0 V/Å. We calculate the electric-field dependence of the band structure and the topological invariant Z2 on the one-bilayer Bi(111) film. To compute the Z2 invariant, we use the Wannier function center (WFC)10,11) and the lattice Chern number (LCN)12,13) because the parity method14) cannot be applied to systems with electric fields. The one-bilayer Bi(111) shows a topological phase transition from the topological insulator phase to a trivial insulator phase under the application of electric fields.

We show the structure of the one-bilayer Bi(111) film and the direction of the applied electric field in Fig. 1(a). The unit cell is a honeycomb lattice, similar to that of graphene, with a buckled structure. We set the length of the side in the cell as 4.54 Å and the buckling height as 1.45 Å, as reported experimentally.3)

We perform fully relativistic density functional calculations using the OpenMX15) code. We use the local spin density approximation (LSDA)16) as the exchange–correlation functional. We use norm-conserving pseudopotentials17) and the linear combination of multiple pseudoatomic orbitals (LCPAO) for wave function expansion.18,19) The cutoff radius is specified as 8.0 Bohr radii and the pseudoatomic orbitals are specified by s3p3d2 with three s-orbitals, three p-orbitals, and two d-orbitals. We set the cutoff energy of 300 Ry, and the k-space sampling points of 13 × 13 × 1 for the reciprocal lattice vectors. We include the spin–orbit interactions by a j-dependent pseudopotential composed relativistically (fully relativistic pseudopotential).20) We neglect changes in the lattice parameters and atomic positions induced by the electric field. The electric field is introduced as a sawtooth potential, and the system is calculated as a one-bilayer slab model. These computational conditions are the same as those in a previous study.9) We implement methods for computing the Z2 invariants by using WFC and LCN in the OpenMX15) code. Z2 = 1 (mod 2) corresponds to the topological insulator, and Z2 = 0 (mod 2) corresponds to the trivial insulator. We compute the Z2 invariant by the two methods applicable to systems without inversion symmetry.

Fig. 1. (Color online) (a) Top view (top) and side view (bottom) of the atomic structure. (b) Brillouin zone of one-bilayer Bi(111).
First, we investigate the electric field dependence of the band structure of the system. One-bilayer Bi(111) has time reversal symmetry $\epsilon(k, \uparrow) = \epsilon(-k, \downarrow)$, and in the absence of electric fields it has the space inversion symmetry $\epsilon(k, \uparrow) = \epsilon(-k, \downarrow)$. Thus, the system becomes doubly degenerate $\epsilon(k, \uparrow) = \epsilon(k, \downarrow)$ at general $k$ points. The application of an electric field causes spin splitting and resolves the degenerate $\epsilon(k, \uparrow) = \epsilon(k, \downarrow)$ for general $k$ points, as well as the degeneracy of eigenvalues $\epsilon(k, \uparrow) \neq \epsilon(-k, \downarrow)$ except for the time-reversal invariant $k$ points $\Gamma : \frac{2\pi}{a} (0, 0, 0)$ and $M : \frac{2\pi}{a} (0.5, 0, 0)$. Here, $k = \frac{2\pi}{a} (k_x, k_y, k_z)$ means $k = k_x \mathbf{G}_1 + k_y \mathbf{G}_2 + k_z \mathbf{G}_3$ where $\mathbf{G}_m (m = 1, 2, 3)$ is a reciprocal lattice vector. Figures 2(a)–2(d) show the electric field dependence of the band dispersion for one-bilayer Bi(111) under fields of $E = 0$, $1.0$, $2.1$, and $2.5$ V/Å, respectively. We confirm electric field-induced spin splitting as shown in Figs. 2(b) and 2(c). The bandgap is decreased from 0.32 to 0 eV when the applied electric field reaches 2.1 V/Å. Then, the bandgap is closed at $k = \frac{2\pi}{a} (0.053, 0.053, 0)$ as shown in Fig. 2(c). Further increasing the applied electric field opens the bandgap, which reaches 0.34 eV at 4.0 V/Å.

Next, we investigate the $Z_2$ invariant of one-bilayer Bi(111) in the absence of an electric field. In a space-inversion symmetric system, the existence of the topological insulator phase can be distinguished by a product of the parity eigenvalues at the time-reversal invariant $k$ points, $\sum_{m} \delta_m \mathbf{G}_m (0, 0, 0), \frac{2\pi}{a} (0, 0.5, 0), \frac{2\pi}{a} (0, 0.5, 0), \frac{2\pi}{a} (0.5, 0.5, 0)$. If the product is negative, $(-1)^{Z_2} = \prod \delta_i$, the system is in a topological insulator phase, and $Z_2 = 1$. The calculated $\delta_i$ are $-1$, $+1$, $-1$, $-1$ respectively, thus we confirm that $Z_2 = 1$ by the product of parity eigenvalues on one-bilayer Bi(111). This result agrees with the previous study. We compute the $Z_2$ invariant of one-bilayer Bi(111) under an applied electric field. Figure 3 shows the $k_y$ dependence of the occupied WFCs ($r_n$) along the $a$-axis. The WFCs are computed by the one-dimension hybrid Wannier functions. The topological insulator phase can be distinguished from the trivial insulator phase by the evolution of the WFC lines which are the $k_y$ dependence of ($r_n$). If the lines show no gap, the system is topological insulator phase with $Z_2 = 1$. Figure 3(a) shows WFCs at $E = 1.0$ V/Å. The WFC lines cross at $k_y = 0, \pi$. Thus, the topological phase is non-trivial and $Z_2 = 1$. Figure 3(b) shows WFCs at $E = 2.5$ V/Å; the WFC lines have gaps, and therefore the system is a trivial insulator with $Z_2 = 0$. According to these results, 2.1 V/Å is the critical electric field strength to induce the topological phase transition from the topological insulator phase to the trivial insulator phase.

We also compute the $Z_2$ invariants by the LCN to validate the results obtained by the WFC. Figure 4 shows examples of the LCN of the system with the applied electric fields of 1.0 and 2.5 V/Å. The filled circles correspond to the LCN of $+1$, filled circles to the LCN of $-1$, and blanks to the LCN of 0. The topological insulator phase can be distinguished from the trivial insulator phase by summation of the LCN in the half Brillouin zone (corresponding to white spaces in Fig. 4). If the summation of the LCN is an odd number, the system is in a topological insulator phase and $Z_2 = 1$. These results are consistent with the results of WFC. We confirm the appearance of a Dirac metal state at the topological phase transition. Figure 5(a) shows the band...
structure at $E = 2.1 \text{V/Å}$. We confirm the Dirac cone at $\mathbf{k} = \frac{2\pi}{a} (0.053, 0.053, 0)$. In the Dirac cone, the Berry flux $\Phi = \oint A \cdot dl$, $A = (u_\mathbf{k} | \partial | u_\mathbf{k})$ becomes $\Phi = \pm \pi$. We investigate the electric field dependence of the Berry flux around $\mathbf{k} = \frac{2\pi}{a} (0.053, 0.053, 0)$ in Fig. 5(b), where the integrated area is one of square plaquettes formed by the $200 \times 200$ k-point mesh. This result indicates the Dirac metal state.

We show the topological phase dependence of the $Z_2$ invariant, and the bandgap in Fig. 6. One-bilayer Bi(111) transitions from the topological insulator phase to the trivial insulator phase via a Dirac metal state. These results are consistent with the topological insulator phase of the system remaining for $E < 0.8 \text{V/Å}$ and with the monotonous decrease of the bandgap for $E < 1.5 \text{V/Å}$. We predicted a strong electric field-induced topological phase transition in one-bilayer Bi(111).

In order to understand the origin of the topological phase transition, we investigate the partial density of states (PDOS) and the wave function around the Dirac point. The topological phase transition is induced by the band inversion of two different characters. We plot the PDOS near the Fermi level in Fig. 7. Comparing these PDOS, the inversion of PDOS is apparent for atoms Bi1 and Bi2 near the Fermi level. Furthermore, we plot the Bloch wave function of the valence band and conduction band at $\mathbf{k} = \frac{2\pi}{a} (0.05, 0.05, 0)$ in Fig. 8. Comparing the wave functions, we confirm the inversion of the wave function; one spreads along the (100) direction and the other along the (110) direction. This inversion of wave functions arises from charge transfer between Atoms Bi1 and Bi2 by the applied electric field. Thus, we demonstrate that the topological phase transition in one-bilayer Bi(111) is induced by the band inversion of the valence and conduction bands.

In summary, we computed the electric field dependence of the bandgap and $Z_2$ invariant of the one-bilayer Bi(111). We predicted the topological phase transitions from a topological insulator phase to a trivial insulator phase for $E > 2.1 \text{V/Å}$ one-bilayer Bi(111). We plotted the PDOS and wave function around the Dirac point, and we could see band character inversion. Thus, we confirmed that the topological phase transition was induced by band inversion in one-bilayer Bi(111). In considering topological-to-trivial switching devices, $E = 2.1 \text{V/Å}$ is a very strong electric field. However, this critical electric field is proportional to spin–orbit interactions, and it could be reduced by alloying atoms with smaller spin–orbit interactions than Bi, such as Sb or As. We confirmed that strained one-bilayer Bi$_{0.5}$Sb$_{0.5}$ shows the topological phase transition at $E = 1.2 \text{V/Å}$.

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