Electric-field-induced $Z_2$ topological phase transition in strained single bilayer Bi (111)

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For controlling critical electric fields of the topological phase transition in a single bilayer Bi(111), we investigated topological phases in a strained system through first-principles calculations. We found a quadratic band touching semimetallic state at tensile strain $\epsilon = 0.5\%$. Around this strain, the topological phase can be switched to a trivial insulator by an infinitesimal electric field. The momentum positions at which Dirac cones appear in the electric-field-induced topological phase transition changed for the strain $\epsilon > 0.5\%$ and $\epsilon < 0.5\%$. Our results indicate that this topological phase transition could be applied to novel spintronic devices.© 2019 The Japan Society of Applied Physics

The bandgap of single bilayer Bi(111) decreases from 0.32 eV to 0.5%. Around this strain, the topological phase can be switched to a trivial insulator by an infinitesimal electric field. The momentum positions at which Dirac cones appear in the electric-field-induced topological phase transition changed for the strain $\epsilon > 0.5\%$ and $\epsilon < 0.5\%$. Our results indicate that this topological phase transition could be applied to novel spintronic devices.© 2019 The Japan Society of Applied Physics

The epitaxial strain can tune the bandgap of single bilayer Bi(111). Density functional calculations predicted that the bandgap is changed and closed by the tensile strain.12–14 In the previous experiment, Bi(111) thin-film formed on a Si (111) and Bi2Te3 substrate shows the lattice constant $a = 4.54$ Å$^2$ and $a = 4.38$ Å$^3$ respectively. It is reported that topological electronic states of Bi(111) thin-films are changed by the epitaxial strain of these different substrate.15

In this study, based on first-principles calculations, we demonstrated that the critical electric field in single bilayer Bi(111) can be reduced by applying a small tensile strain $\epsilon = 0.5\%$. First, we investigated the bandgap in strained systems. We found a critical strain of bandgap closing and a quadratic band touching (QBT) semimetallic state. We computed $Z_2$ invariants of two different insulator phases that appear under strain and confirmed that both are $Z_2$ topological insulator phases. We also computed the $Z_2$ topological phase in strained systems under applied electric fields. Unlike in our previous studies, we found that the topological phase transition was induced by small electric fields for tensile strain of $\epsilon < 0.5\%$. The momentum positions at which Dirac cones appear in the electric-field-induced topological phase transition changed for the strain $\epsilon > 0.5\%$ and $\epsilon < 0.5\%$. Figure 1 shows the structure of a single bilayer Bi(111). Two atoms in the unit cell of a hexagonal lattice are set. We optimized the buckling height $d$ with the strained lattice constant $a$. We define the tensile strain as $\epsilon = (a - a_{\exp})/a_{\exp}$, where $a_{\exp} = 4.54$ Å is an experimental lattice constant and the buckling height is $d_{\exp} = 1.45$ Å. This strain changes the buckling height. The bandgap of other hexagonal lattice systems like a graphene and silicone can be tuned by the changing buckling height. Therefore, we expect that the bandgap of single bilayer Bi(111) is related to the buckling height $d$.

We performed density functional calculations using the OpenMX code.17 We used the local spin density approximation18,19 as the exchange correlation functional. We used norm-conserving pseudopotentials20 and the linear combination of multiple pseudoatomic orbitals21,22 for wave function expansion. We set the pseudoatomic basis as Bi8.0-s3p3d2; this indicates a cutoff radius of 8.0 Bohr and pseudoatomic orbitals as three s-orbitals, three p-orbitals, and two d-orbitals. Spin-orbit interactions were included by a $j$-dependent pseudopotential composed relativistically (fully relativistic pseudopotential),23 where $j$ is the total angular momentum. We set $k$-space sampling points of $13 \times 13 \times 1$ for reciprocal lattice vectors and cutoff energy of 300 Ry. Electric fields were introduced as sawtooth potentials24,25 and we assumed that the lattice parameters and atomic positions were not changed by electric fields.

For confirming $Z_2$ topological phases of the system, we used the lattice Chern number method.26,27 The $Z_2$ topological phase is determined by a $Z_2$ invariant.28 $Z_2 = 1$ corresponds to a topological insulator phase, and $Z_2 = 0$ corresponds to a trivial insulator phase. The lattice Chern number method computes the $Z_2$ invariant as $Z_2 = 1/2\pi \int_{\text{Brillouin zone}} \langle \mathbf{F} \cdot \mathbf{k} - \mathbf{F} \mathbf{k} \rangle$ (mod 2) on a half Brillouin zone $-G_1/2, G_1/2 \bigotimes [0, G_2/2]$, where $\mathbf{A}_\mathbf{k} = \langle u_{\mathbf{A}} \rangle \partial_{\mathbf{k}} |u_{\mathbf{A}}\rangle$ is the Chern curvature and $\mathbf{F} = \nabla \times \mathbf{A}$ is called the Berry curvature. This method can be applied to the system with the broken spatial inversion symmetry. We also use the parity method29 for computing $Z_2$ invariant of the system without electric fields. The parity method computes the $Z_2$ invariant as $\prod_{i=1}^{n} \delta_i = (1)^{2i_1}$, where $\delta_i = (i=1, 2, 3, 4)$ is the parity sign on $k$ time-reversal-invariant points $(I_1, 2\pi/a(0, 0, 0), I_2, 2\pi/a(0.5, 0, 0), I_3, 2\pi/a(0.5, 0.5, 0)$, and $I_4, 2\pi/a(0.5, 0.5, 0))$. Here, $\mathbf{k} = 2\pi/a(k_1, k_2, k_3)$ implies that $\mathbf{k} = k_1 \mathbf{G}_1 + k_2 \mathbf{G}_2 + k_3 \mathbf{G}_3$, where $\mathbf{G}_m (m = 1, 2, 3)$ is a reciprocal lattice vector. We implemented these two methods in OpenMX code.17
Fig. 1. (Color online) Structure of a single bilayer Bi(111). We optimized the buckling height with a strained lattice constant.

First, we optimized the buckling height when the lattice constant is strained as $-5\% < \epsilon < +5\%$ without an electric field. The buckling height decreases as the lattice constant increases. It is $d = 1.75\,\text{Å}$ at $\epsilon = -5\%$ and $d = 1.47\,\text{Å}$ at $\epsilon = +5\%$. When we optimize the atomic structure at $a_{\text{exp}}$, the obtained buckling height is $1.63\,\text{Å}$, larger than the experimental parameter $d_{\text{exp}} = 1.45\,\text{Å}$. This is because our calculated system has a single bilayer, whereas seven or more Bi (111) bilayers were formed on Si(111) experimentally.

Next, we investigated the band structure for the strain of $-5\% < \epsilon < +5\%$ without electric fields. Figure 2(a) shows the bandgap for various strains without electric fields. For $\epsilon = -5\%$, the bandgap is 0.53 eV and decreases monotonically with increasing strain. This bandgap decreasing is originated from a change in buckling height, $d = 1.75\,\text{Å}$ for $\epsilon = -5\%$ and $d = 1.61\,\text{Å}$ for $\epsilon = 0.5\%$. At $\epsilon = \epsilon_{\text{QBT}} = 0.5\%$, the bandgap is closed at the $\Gamma$ point by the spin-orbit interaction, and the system shows a semimetallic QBT state, as shown in Fig. 2(b). Upon further increasing the strain, the bandgap is opened and reaches 0.47 eV at $\epsilon = +5\%$. This bandgap increasing can be understood by changing spin–orbit coupling induced by localization of wave functions. We confirmed the mechanism of the bandgap by calculating band structures without spin–orbit coupling. On turning off spin–orbit coupling, the bandgap is opened for $\epsilon < \epsilon_{\text{QBT}}$, while the bandgap is closed for $\epsilon > \epsilon_{\text{QBT}}$.

We calculated $Z_2$ invariants by the parity method and lattice Chern number method. In most cases, the strain induced $Z_2$ topological phase transition occurs when the bandgap is closed. However, in the present case, the system always has $Z_2 = 1$; therefore, strained single bilayer Bi(111) preserves the $Z_2$ topological insulator phase. Figure 2(c) shows the wave function and parity sign at the $\Gamma$ point at around the critical strain. We can confirm band inversion at the $\Gamma$ point by investigating the shapes of the wave functions on the valence band and conduction band; however, the parity sign of both bands is equivalent, and therefore, the result of computing $Z_2$ invariants does not change. This result may suggest that another topological invariant instead of the $Z_2$ invariant is changed by the strain. Both of insulating phases can be characterized by the topological invariant corresponding to a combination of spin and symmetry operators, as in a topological crystalline insulator characterized by a mirror Chern number. To confirm this, we require further theoretical investigations.

We investigated the electric-field-induced $Z_2$ topological phase transition. Figure 3(a) shows a topological phase diagram of strained systems under electric fields. The topological insulator phases are switched to trivial insulator phases by electric fields, as reported in our previous study. For $\epsilon < \epsilon_{\text{QBT}}$, the critical electric field is drastically enhanced by compressive strain ($\epsilon < 0$) compared to tensile strain ($\epsilon > 0$) for $\epsilon > \epsilon_{\text{QBT}}$. An important result is the fact that the topological phase of the system around $\epsilon = \epsilon_{\text{QBT}}$ can be switched by an infinitesimal electric field; therefore, we can achieve topological phase switching by realistic electric fields if we use these strain states.

The Dirac cones appeared in the electric-field-induced $Z_2$ topological phase transition are different between $\epsilon > \epsilon_{\text{QBT}}$ and $\epsilon < \epsilon_{\text{QBT}}$. When the $Z_2$ topological phase changes in the two-dimensional system, Dirac semimetals appear. Figure 3(b) shows the band structure at the critical electric field for various strains. For $\epsilon < \epsilon_{\text{QBT}}$, Dirac cones appear at the $\Gamma$ point [single Dirac cone (SD) state in the phase diagram Fig. 3(a)] when the bandgap closes under the applied electric field. Two unoccupied bands and two valence bands are degenerate at the $\Gamma$ point in the SD state. In contrast, for $\epsilon > \epsilon_{\text{QBT}}$, six Dirac cones appear on the $\Gamma$–$K$ line [multiple Dirac cone (MD) state in the phase diagram Fig. 3(a)] as in our previous study. One unoccupied band and one valence band are degenerate on the every Dirac cone in the MD state. The appearance of these Dirac cones are closely linked to the
QBT state. The QBT is parabolically band crossing at the Fermi energy\(^{30,31}\) and its Berry flux \(\Phi = -i \int \mathbf{k} \cdot \mathbf{A} \) is 0 at this point in the case of accidental band crossing. The QBT in the present system appears at \(\Gamma \) point [QBT in the phase diagram Fig. 3(a)]\(^{\text{36}}\), two unoccupied bands and two valence bands are degenerate. This QBT can split into several Dirac cones with \(\Phi = \pm \pi\) with broken spatial inversion symmetry while preserving the total Berry flux \(\Phi = 0\). In the SD state, we confirm \(\Phi = 0\) at \(\Gamma\) point because Dirac cones are degenerate and both Berry flux \(\Phi = \pm \pi\) of Dirac cones cancel each other out, but its band dispersion is linear clearly. In the MD state, we confirm \(\Phi = -\pi\) for three Dirac cones and \(\Phi = \pi\) for three Dirac cones.\(^{\text{36}}\)

In summary, we investigated the strains and electric field effects of single bilayer Bi(111) through a first-principles study. We computed the bandgap and topological phase against the strain and found that the bandgap was closed and the quadratic band touching semimetallic state appeared at \(\Gamma\) point for \(\epsilon = \epsilon_{\text{QBT}}\); however, the \(\Gamma_2\) topological phase did not change. We also investigated the \(\Gamma_2\) topological phase under applied electric fields. The topological phase can be switched by an infinitesimal electric field near \(\epsilon = \epsilon_{\text{QBT}}\), and we achieve switching of the \(\Gamma_2\) topological phase of single bilayer Bi(111) by reasonable electric fields. For \(\epsilon > \epsilon_{\text{QBT}}\), the electric-field-induced topological phase transition occurs as described in our previous study;\(^{10}\) six Dirac cones appear on the \(\Gamma-K\) line. On the other hand, for \(\epsilon < \epsilon_{\text{QBT}}\), the topological phase transition occurs differently; degenerate Dirac cones appear at the \(\Gamma\) point. This difference may be related to the experimental study of Bi(111) thin-film showing different surface states under a tensile strain.\(^{15}\)

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Fig. 3. (Color online) (a) Topological phase diagram and critical electric field (data points) for various strains. (b) Band structure at critical electric field for various strains. For example, there is a single Dirac cone state (SD) at \(\epsilon = 0.6\%\) and \(E = 2.6\) V Å\(^{-1}\) and a multiple Dirac cones state (MD) at \(\epsilon = 4.4\%\) and \(E = 2.6\) V Å\(^{-1}\). Momentum positions of Dirac cones changed for \(\epsilon < \epsilon_{\text{QBT}}\) and \(\epsilon > \epsilon_{\text{QBT}}\).