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Outline of this thesis

Various unique spin structures have been found in the interfaces and surfaces of Rashba systems and topological insulators with the SOI. Therefore, in this thesis, we investigate these unique spin states and theoretically find novel states in the surfaces and multilayers focusing on its symmetry and topology.

In Chapter 3, we studied the non-Rashba surface states of the Tl/Si and the Bi/Si. On the Tl/Si surface the spin splitting at the $\bar{K}$ point gives rise to spin directions normal to the surface. In addition, on the Bi/Si surface there is a "peculiar" Rashba splitting at the $\bar{K}$ points. It is called peculiar because the $\bar{K}$ points are not time-reversal invariant, which is different from the conventional Rashba splitting appearing only around time-reversal invariant $\boldsymbol{k}$ points. Furthermore, at the $\bar{M}$ point in the Bi/Si surface, the spin texture is not of the Rashba type, but is similar to that of the Dresselhaus type. Such unconventional systems motivate us to study new spin properties in hybrid systems consisting of materials with non-Rashba SOI (shown in Chapter 4). We derived effective nearest-neighbor tight-binding Hamiltonians for the surfaces of these non-Rashba surfaces by taking into account the crystal symmetries. The energy band of the Tl/Si model has non-Rashba splitting and the spin direction for each band is perpendicular to the crystal surface at the $\bar{K}$ point. The energy band of the Bi/Si model has peculiar Rashba splitting not at time-reversal invariant point but at the $\bar{K}$ point. Our results of the model calculation qualitatively agree with the experimental results. We identified the non-Rashba term which is responsible for the non-Rashba spin splitting in the Tl/Si, and such term does not exist in Rashba systems even in the Bi/Si model. Systems having non-Rashba or peculiar Rashba SOI may have novel spin properties and interesting physical phenomena, for example, the persistent spin helix and the Edelstein effect. Because in the Tl/Si, the spin direction around $\bar{K}$ point is normal to the crystal surface can affect the phenomena which depends on spin directions of the SOI. Therefore, we applied the theorey of the Edelstein effect to the Tl/Si model, and we find that the out-of-plane spin does not appear in the Edelstein effect in this model because the crystal symmetries prohibit the out-of-plane spin polarizaiton. In contrast, we applied the persistent spin helix theory to the Tl/Si model, and we find in-plane spin helix which is different from the out-of-plane spin helix in the previous work introduced in section 2. Given these factors, the non-Rashba system can be applied to many physical phenomena, with unconventional types of spin direction. Furtheremore, the symmetries of the Tl/Si model is similar to the transition metal dichalcogenide monolayers, which are atomically thin semiconductors of the type MX_2, with M being a transition metal atom (Mo, W, etc.) and X a chalcogen atom (S, Se, or Te). Thus, there are many materials having the out-of-plane spins in the spin spliting by SOI, which means that junctions and multilayers of the non-Rashba system have various choices of real materials.

In Chapter 4 we studied the junction between the two surface regions which have different signs of the SOI parameters in the Tl/Si system and in the Bi/Si system. We considered two cases for the direction of the junction between two regions. In these junction models, the SOI parameter (λ_z in the Tl/Si and λ_y in the Bi/Si) is set as $+\lambda$ and $-\lambda$ in the two regions, respectively. As a result, we numerically found bound states at the these junctions. From the lattice model we found that the spins of the bound states in the Bi/Si model is out-of-plane, which is in contrast with the in-plane spin direction in the bulk. Nevertheless, from the continuum model we cannot reproduce the existence of the bound states. To realize this junction, we proposed BiTeI, because the SOI of our junction is similar to the Rashba SOI, and by changing the stacking order of atomic layers of BiTeI it might be possible to achieve different signs of Rashba SOI.

In Chapter 5 we introduced the multilayer of TI, consisting of alternating layers of two TIs and a NI. In this model, we found that the phase diagram contains the TNS phase when the top surface and the bottom surface states of the neighboring TI layers hybridize strongly than that of the same TI layer. The TNS phase has a nodal line protected by the "internal", inversion and time-reversal symmetries, which is different from the conventional mechanism of nodal lines. Surprisingly, there nodal surface exist even when the inversion symmetry is broken. Namely, the nodal surface is protected by the mirror symmetry caused by high symmetry of this system. Next, we studied the nature of TNS phase by perturbing the system. We added a warping term in the TI multilayer to break symmetries in three patterns with different combinations of the warping terms. We found Dirac semimetal, nodal line semimetal and nodal surface semimetal phases in these multilayers. The Dirac points and the nodal line are protected by the internal symmetry, and the difference between the Dirac semimetal and the nodal line semimetal phases is whether the internal symmetry is present. The nodal-surface semimetal phase contains the gapless points forming six closed surfaces. There are six degeneracy points at $k_z = 0$ plane, which is caused by the internal symmetry. Additionally, when we break the inversion symmetry by modulating the hybridization D, six nodal lines and nodal surfaces appear, respectively. The six nodal lines are also protected by the mirror symmetry, and the nodal surface is topologically characterized as zeros of the Pfaffian of a product between the Hamiltonian and a constant matrix. Furthermore, when we break the both internal and inversion symmetries, nodal lines still survives and they have a topological origin. Finally, we found a peculiar surface states in the TI multilayer and the multilayer of non-Rashba type. We analyzed the surface states in the TI multilayer by using an eight-band model. The surface states are originated from an absence of hybridization between unit cells. The surface states are similar to the bound states in the zigzag graphene ribbon. In the zigzag graphene ribbon, the bound states are constructed only from the wavefunctions at one of the two sublattices.

The nodal line has been actively studied recently. In systems such as Ca, Sr, and Yb without the SOI, and $TlTaSe_2$ with the SOI, one finds "drumhead surface states" in those surfaces, in Ca(110), Sr(110), Yb(110), and a surface of $TlTaSe_2$. Surface states connecting between the gapless points exist near the Fermi level. In the previous work, the authors found that large Rashba splitting may be caused by the nodal line, such as in Bi/Sr(111). The nodal lines near the Fermi level enhance the Rashba splitting at the surface due to the bulk polarization, coming from the π Zak phase. In addition, Bi/Ag(111), Ag also has the nodal line, and the drumhead surface states from the nodal line hybridize the Rashba splitting bands at the surface and may enhance the Rashba splitting. These effect from the nodal line are interesting because the bulk band affects the surface bands. Additionally, it is an interesting issue to investigate the difference between the conventional drumhead surface states and surface states in the lattice model of the model A, because they have different origins of the nodal line. In addition, in the previous work, there are an unconventional spin texture of the surface states, which is distinct from the spin-momentum-locked texture of Dirac surface states in conventional topological insulators. In the multilayer of the model C', D and D', the inversion symmetry is broken so that the energy band of the nodal surface has spin splitting. In these models, we expect that unconventional spin texture exists in the bulk bands and surface states, coming from the nodal surface, which is unlike the conventional TIs and that of the TlTaSe$_2$. Furtheremore, we also expect that such unusual spin texture in the bulk band and in the surface will offer unique possibilities in spintronics applications. The Dirac semimetal and nodal line semimetal having unconventional origins and the nodal surface semimetal with the SOI have much room for further research.

To summarize the whole results, modulation of the SOI allow various unique spin structures and electronic band structures due to symmetry and topology of the system. By designing nanostructures such as multilayers, junctions and interfaces using various materials with the SOI, one can have broad possibilities for spin properties and novel electronic structures, and will offer us promising possibilities for spintronics applications.