Interface-induced Topological Insulator Transition in GaAs/Ge/GaAs Quantum Wells

Dong Zhang$^1$, Wenkai Lou$^1$, Maosheng Miao$^2$, Shou-cheng Zhang$^3$ and Kai Chang$^4$

$^1$SKLSM, Institute of Semiconductors, Chinese Academy of Sciences, P.O. Box 912, Beijing 100083, China
$^2$Materials Research Laboratory and Materials Department, University of California, Santa Barbara, California 93106-5050, USA and
$^3$Department of Physics, Stanford University, Stanford, CA 94305

We demonstrate theoretically that interface engineering can drive Germanium, one of the most commonly-used semiconductors, into topological insulating phase. Utilizing giant electric fields generated by charge accumulation at GaAs/Ge/GaAs opposite semiconductor interfaces and band folding, the new design can reduce the sizable gap in Ge and induce large spin-orbit interaction, which lead to a topological insulator transition. Our work provides a new method on realizing TI in commonly-used semiconductors and suggests a promising approach to integrate it in well developed semiconductor electronic devices.

PACS numbers: 71.70.Ej, 75.76.+j, 72.25.Mk

Time-reversal invariant topological insulators (TIs) have aroused intensive interests in the past years, with tantalizing properties such as insulating bulk, robust metallic edge or surface modes and exotic topological excitations, and potential applications ranging from spintronics to quantum computation.[1–15] Despite these successful progresses, the topological insulator materials are still limited in the narrow gap materials containing heavy atoms, e.g., HgTe,[3, 16, 17] Bi$_2$X$_3$ (X=Se, Te,...)[8–11], transition metal oxide heterostructure[16] and Heusler compounds[12, 17]. These materials are often very different from conventional semiconductor materials in structures and properties and are hard to be integrated in current electronics devices and are based on well developed semiconductor fabrication technologies.

Although there are theoretical predicts about realizing TI states in graphene,[3, 16, 18, 19] the main obstacle is the weak intrinsic spin-orbit interaction (SOI) of carbon atoms. Here, instead of searching new TI materials with exotic structures and chemical elements, we take a totally different route: driving the commonly used semiconductors into TI states by using the intrinsic electric field and the strains. The difficulty of this approach lies in the fact that most of the commonly used semiconductors, such as Si, Ge, GaAs and many others usually possess sizable band gaps and do not have strong enough SOI. Furthermore, group IV elements such as Si and Ge have indirect band gap, posing extra difficulty in realizing TI. Inspired by recent theoretical works that the normal insulator can be driven into a TI by an external electric field, our approach is to impose huge electric field by deliberately designed heterostructures. Recently, an interesting way of realizing topological insulating phase in a p-type GaAs quantum well by two-dimentional superimposed potentials with hexagonal symmetry was proposed.[21] Different to that work, our approach rely completely on the material engineering at the atomic level.

Since commonly-used semiconductors, e.g., Si, Ge, GaAs, possess sizable bandgap ranging from 0.8eV to 1.4eV, a huge electric field is required to closing bandgap and even invert the conduction and valence bands. Such huge electric field can not be generated utilizing the gate technique. However, recent technical advances in the atomic-scale synthesis makes it possible to fabricate high quality semiconductor and oxide heterostructures. It provides us abundant opportunities to create novel quantum states and emergent phenomena at the interfaces by reconstructing charge, spin and orbital states. Very recently, a new way to exploring topological insulating phase in semiconductors was proposed utilizing strong piezoelectric effect at the interface between GaN and InN.[22] The strain between these material results in a huge polarization and electric field cross the interfaces. This huge electric field not only can invert the conduction and valence bands, but also generate strong Rashba SOI, eventually drive the system into topological insulating phase. Strong strain (∼10%) in this system may cause two opposite effects, since it drives the system into topological insulating phase; but the release of the strain can also induce defect, vacancy and dislocation in the samples, the density of these defects increases rapidly as the thickness of InN layers increases, making the sample growth and fabrication very challenging. To overcome this obstacle, it would greatly advance the field if one can realize the topological insulator in lattice-matched common semiconductors.

Ge and GaAs are both important materials for microelectronic and optoelectronic device applications. Very recently, Ge/GaAs heterostructures realized by epitaxy methods paved the way to heterostructure based devices utilizing the band offsets, quantum size effects and band structure modifications by electric fields. Ge/GaAs quantum structures promise the dramatic mobility increase needed for power saving electronics.[23, 24] Ge/GaAs interfaces with exceedingly small lattice mismatch posses many advantages over the strained interface. Ge layers grown on GaAs substrate were studied because of their widespread applications
FIG. 1: (color online) (a) Schematic of the structure of a ultrathin Ge layer sandwiched by thick GaAs layers (the upper-left panel). The upper-right panel amplifies the atomic configuration of the GaAs/Ge/GaAs quantum well containing four bilayer Ge. Notice that the Ga and As atoms locate at the opposite interfaces which leads to a charge accumulation schematically shown in the left panel. (b) The Brillouin zone (BZ) of bulk Ge and the folded BZ of GaAs/Ge/GaAs QW along the [111] crystallographic direction. (c) The charge accumulation at two opposite interfaces obtained from the first-principle calculation. The red and green isosurfaces describe the positive and negative charge accumulations at opposite interfaces.

In order to demonstrate the TI transition in GaAs/Ge/GaAs, we employ two complementary approaches, the first principles methods based on density functional theory (DFT) and the multi-band k·p theory. In the first approach, the GaAs/Ge/GaAs structure is modeled by a series of supercells consisting of 15 atomic bilayers in which the thickness of Ge layer varies from 1 bilayer to 6 bilayers. (periodicity requires that the total number of atomic layers be even). Because of the key importance of the band gaps, we use a hybrid functional in Heyd-Scuseria-Ernzerhof (HSE) scheme, an approach that has been proved to yield band gaps in good comparison with experimental values for majority of semiconductor materials, as implemented in the VASP program. Using a standard mixing parameter of 0.25, we found the band gaps of GaAs and Ge to be 1.08 and 0.73 eV (Ref. 35). The lattice parameters $a=b=c$ are found to be 5.655 Å for GaAs and 5.657 Å for Ge. On the other hand, SOI is not included in our DFT calculations because of the exceedingly large computing demand while combining HSE and SOI. Instead, we adopt a 30-band k·p Hamiltonian with SOI and apply it to the GaAs/Ge/GaAs QWs. The 30-band k·p model was used to calculate the band structure of commonly-used semiconductors in whole Brillouin zone.

In solar cells, metal-oxide-semiconductor field-effect transistors, millimeter-wave mixer diodes, temperature sensors, and photodetectors.

Considering a GaAs/Ge/GaAs quantum well (QW) grown along the polar direction [111] (see Fig. 1), a large electric field can be induced in the sandwiched Ge layer. In GaAs/Ge/GaAs QW, one interface consists of As-Ge bonds and the other consists of Ga-Ge bonds. Because each As contains five electrons whereas Ga contains only three, charge will transfer from As-Ge side to the Ga-Ge side and a large electric field will be created and imposed on the Ge layer. The electric field will shift the electron and the hole states to the left and right sides of the QW and reduce their energy difference (band gap), and may eventually invert their order. In addition, the electric field also induces a considerably large Rashba SOI.

FIG. 2: (color online) (a) Band structures of GaAs/Ge/GaAs sandwiched structures with different Ge portions obtained from the first-principles HSE calculations. From left to right, two Ge bilayers, four Ge bilayers and four Ge bilayers with 3% in-plane tensile strain. (b) The bandgap (purple-diamond line) and the inner polarization field strength (blue-square line) as functions of the number of Ge bilayers. (c) The variation of bandgap $\Delta E_g = E_{g}^{strain} - E_{g}$ as a function of in-plane strain.
The proposed GaAs/Ge/GaAs structure is shown schematically in Fig. 2(a), together with an inset showing the atomic structure of the GaAs/Ge interfaces along the (111) growth direction. As is well known, Ge is an indirect semiconductor with the VBM at the Γ point and the CBM at the L point. While growing a heterojunction along (111) direction, the symmetry are broken and the bands are folded along the Γ-L direction (see Fig. 2(b)). As a result, the CBM at the L points in bulk Ge is folded to the Γ point and the Ge thin layers growing in (111) direction possesses a direct gap at Γ. The band folding is non-trivial, as we will show below in both DFT calculation and $k \cdot p$ model. The breaking of the cubic symmetry also leads to a strong coupling between the electron and the hole states, which is essential for the TI transition.

Fig. 2(a) presents the HSE band structures of GaAs/Ge/GaAs QW with 2 and 4 bilayers of Ge. The two-Ge-bilayer QW has a gap of 0.8 eV that is comparable to the direct gap of Ge at Γ point. At four Ge bilayers, the gap decreases to 0.3 eV. The large remaining band gap is the result of strong quantum confinement effect, which will decrease with the increasing Ge layer thickness. In both these cases, the band structures still display normal order in the sense that the heavy hole (HH) and light hole (LH) states are degenerate at the Γ point ($\Gamma_5$) and are lower in energy than the electron state ($E$, $\Gamma_1$). As a matter of fact, our HSE calculations show that the charge field itself can not drive the system into inverted bands. As shown in Fig. 2(c), the band gap keep decreasing but remain positive with up to 6 bilayers of Ge.

The driving force of the decreasing band gap is the strong electric field imposed by the charges located at the two interfaces in GaAs/Ge/GaAs QW (see Fig. 2(c)). In principle, the strength of the electric field should not change with increasing thickness of the Ge layer. However, because of the finite size of our supercell, the actual model in the HSE calculations are a GaAs/Ge superlattice, in which the GaAs region is much thicker than the Ge region. For that reason, the electric field slightly goes down with increasing Ge thickness. This feature is well captured by the HSE calculations as shown in Fig. 2(c). While the QW contains more than 4 Ge bilayers, the HSE calculations shows that the electric field goes down dramatically. It decreases from 12.5 MV/cm for 4 Ge bilayer to 8.5 MV/cm for 6 Ge bilayer. The decreasing electric field is a result of charge transfer from Ga-Ge interface to As-Ge interface, which weakens the driving force toward band inversion.

While the bands of GaAs/Ge/GaAs QW remains in normal order with increasing Ge thickness, we found that a slight tensile strain is enough to drive the system into inverted bands. As shown in the upper right panel of Fig. 2(a), the system exhibits an inverted band structure, in which $\Gamma_5$ states are 0.1 eV higher than the $\Gamma_1$ state for 4 Ge bilayer with 1% tensile strain, and 0.2 eV for 2% strain. The actual band inversion can happen under a much smaller strain. This slight tensile strain can be realized by doping In atoms into GaAs host material, bending the sample, or growing the heterostructures on a substrate with larger lattices. In Fig. 2(b), the states around Γ point are still denoted as E, HH and LH according to its energy order, which is different to the notation used in previous works. Such an inverted band structure is a signature of the transition to a TI state. Similar to bulk Ge, the effect of the strains on the band gaps of GaAs/Ge/GaAs QW are quite strong. As shown in Fig. 2(c), the band gap can change for about 0.2 eV with 2% compressive and tensile strains, providing us an effective way to control the TI transition.

Although the HSE band structure calculations show that the combination of the strong electric field and a modest strain can invert the bands of GaAs/Ge/GaAs QW at Γ point, it is not sufficient to prove the TI transition. In order to show the TI transition, both band inversion and the SOI should present. The calculation of band structure at the hybrid functional level with SOI for a QW system is extremely demanding on computing resources. We therefore take another approach by constructing a multi-band $k \cdot p$ model Hamiltonian. The parameters of the model are carefully calibrated with HSE calculations. Comparing with HgTe system, there are more valence bands involved in interacting with the electron state at the Γ point. We find that the inclusion of 30 bands in total is sufficient to describe complicated interband coupling at the Γ point of the Brillouin zone of GaAs/Ge/GaAs QWs. The most important states near the bandgap are the spin-up and spin-down electron states ($|E, \uparrow\rangle$ and $|E, \downarrow\rangle$), the spin-up and spin-down heavy hole ($|HH, \uparrow\rangle$ and $|HH, \downarrow\rangle$) states. We would like to emphasize that the electron and heavy hole subbands ($|E, \uparrow\rangle$ and $|HH, \uparrow\rangle$) denote only the dominant components of the lowest conduction and highest valence subbands and are mixed with electron and heavy- and light-hole states due to the interband coupling in the $k \cdot p$ theory.

By applying the $k \cdot p$ theory, we first confirm the band inversion in the GaAs/Ge/GaAs QW system. The numerical simulation shows that the inversion happens when the thickness of Ge layer is larger than 18Å and the QW is subject to about 0.5% tensile strain. This corresponds to about 4 Ge bilayers and is in excellent agreement with the HSE results. The inverted bands are shown in Fig. 2(a), the electron $\Gamma_5$ state is lower in energy than the valence $\Gamma_1$ state. Clearly, it is the result of the fact that the highest valence subbands $|HH, \uparrow\rangle$ are heavily involved in the coupling with electronic subbands $|E, \uparrow\rangle$ near the Γ point.

Spin-orbit interaction is essential in the transition to a TI state. The intrinsic SOIs in both Ge and GaAs are not strong enough to creating TI states. We found that the large interface electric field induces a consider-
ably large Rashba SOI splitting from the 30-band $k\cdot p$ theory for electron and hole states ($\sim$2–15meV, see the inset of Fig. 3(a)), respectively. The magnitude is comparable with that in HgTe QWs. This large Rashba SOI in GaAs/Ge/GaAs QW is a nature results of the strong electric field and can be derived from the multiband $k\cdot p$ theory. No fitting parameters are required except the strength of the electric field, which is adopted from the HSE DFT calculation (see Fig. 2(b)). The strong Rashba SOI in QWs provides a controllable approach to creat TI states in GaAs/Ge/GaAs QWs. The essential feature of 2D TI is the existence of the helical edge states near the boundary of such 2D QWs. The experimental detection the aforementioned edge states in GaAs/Ge/GaAs Hall can be performed in the standard four terminal measurements. The edge states can be observed at the minigap opened between the E1 and the HH1 bands. According to our calculations using the $k\cdot p$ model, this minigap can be as large as 15 meV, which is already larger than the similar minigap in InAs/GaSb QW system, another 2D TI in which the edge states has recently been observed.

We downfold the 30 band model Hamiltonian to an effective two-dimensional (2D) four-band Hamiltonian expressed in the above four basis ($|E, \uparrow\rangle$ and $|HH, \uparrow\rangle$). The exact form and the derivation process of the four-band effective 2D Hamiltonian can be found in the supplementary information. The contributions from the lowest and highest ten subbands are included in this four-band reduced Hamiltonian via the Löwdin perturbation theory. The explicit expression of four-band effective two-dimensional Hamiltonian Hamiltonian in the basis $|E_1, \uparrow\rangle$, $|HH, \uparrow\rangle$ is

$$
H_{4\times4}^{eff} = \begin{bmatrix}
E_0 + E_1 k_x^2 & A_1 k_+ & 0 & 0 \\
A_1^* k_- & H_0 + H_1 k_x^2 & 0 & 0 \\
0 & 0 & E_0 + E_1 k_x^2 & -A_1 k_- \\
0 & 0 & -A_1^* k_+ & H_0 + H_1 k_x^2
\end{bmatrix}
$$

where $k_x$ denotes the in-plane momentum, and $k_\parallel = k_x \pm i k_y$, the relevant parameters $E_0 = -0.19808$ eV, $E_1 = 0.43810$ eV$\cdot$Å$^2$, $H_0 = -0.19153$eV, $H_1 = -0.20810$eV$\cdot$Å$^2$, $A_1 = 0.028510$eV$\cdot$Å.

From the above four-band effective Hamiltonian, we can start to study the topological insulator transition in such 2D QWs. The essential feature of 2D TI is the existence of the helical edge states near the boundary of 2D TI sample. We consider a quantum wire structure with a width of 1000 Å. The thickness along the (111) growth direction consists of a Ge layer of 18 Å, sandwiched by two 200 Å GaAs layers. Fig. 3(b) shows the band structure of the above quantum wire together with the density distribution of a Kramers pair of edge states. As shown in the figure, the new energy branches appear and sweep across the bulk gap, these states are highly localized near the edge of the quantum wire. The spin-up and spin-down edge states with the same in-plane momentum $k = 0.01$ Å$^{-1}$ along the quantum wire localize at the opposite edges, in contrast to the chiral edge states in the integer quantum Hall effect, where the spin-up and spin-down electron with the same in-plane momentum localize at the same edge. The presence of these helical edge states clearly demonstrates the TI transition in this two-dimensional GaAs/Ge/GaAs QW system.
considerable advantage over other TI systems including graphene \[3\], HgTe QW, \[4, 5\] the Bi chalcogenides \[9\] and the Heusler compounds \[12, 17\]. GaAs/Ge/GaAs sandwiched structures are readily to be integrated with conventional semiconductors which are already extensively used in electronic devices \[23–31\]. The imposed electric field can be controlled by applying extra electric field or by inducing holes or electrons into the QW region via a gate voltage, providing us a direct way of manipulating the TI transition in the device. The transition point can also be adjusted by well developed semiconductor techniques such as alloying and doping.

This work was supported by the NSFC Grants No. 10934007 and the grant No. 2011CB922204 from the MOST of China, and M.S.M. is supported by the MRS-SEC program (NSF-DMR1121053) and the ConvEne-IGERT Program (nsf-dge 0801627). S.C.Z. is supported by the DARPA Program No. N66001-12-1-4034. KC would like to thank Prof. Bangfen Zhu, Qikun Xue, Zhong Fang, Xi Dai for their valuable discussions.

[1] M. Z. Hasan, and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
[2] X. L. Qi, and S. C. Zhang, Rev. Mod. Phys. 83, 1057 (2011).
[3] C. L. Kane, and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005).
[4] B. A. Bernevig, T. L. Hughes, and S. C. Zhang, Science 315, 1757-1761 (2007).
[5] M. Konig, et al. Science 318, 766-770 (2007).
[6] C. X. Liu, T. L. Hughes, X. L. Qi, K. Wang, and S. C. Zhang, Phys. Rev. Lett. 100, 236601 (2008).
[7] I. Knez, R. -R. Du, and G. Sullivan, Phys. Rev. Lett. 107, 136603 (2011).
[8] L. Fu, C. L. Kane, and E. J. Mele, Phys. Rev. Lett. 98, 106803 (2007).
[9] D. Hsieh, et al. Nature 452, 970-974 (2008).
[10] Y. L. Chen, et al. Science 325, 178-181 (2009).
[11] Y. Xia, et al. Nature Phys. 5, 398-402 (2009).
[12] S. Chadov, et al. Nature Mater. 9, 541-545 (2010).
[13] H. Lin, et al. Nature Mater. 9, 546-549 (2010).
[14] M. Franz, Nature Materials 9, 536 (2010).
[15] K. Yang, et al. Nature Mater. 11, 614-619 (2012).
[16] D. Xiao, W.G. Zhu, Y. Ran, N. Nagaosa, and S. Okamoto, Nature Commun. 2, 596 (2011).
[17] D. Xiao, Y. Yao, W. Feng, J. Wen, W. Zhu, X. Q. Chen, G. M. Stocks, and Z. Zhang, Phys. Rev. Lett. 105, 096404 (2010).
[18] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, Rev. Mod. Phys. 81, 109 (2009).
[19] Z. Qiao, W. K. Tse, H. Jiang, Y. Yao, and Qian Niu, Phys. Rev. Lett. 107, 256801 (2011).
[20] W. Yang, K. Chang, and S. C. Zhang, Phys. Rev. Lett. 100, 056602 (2008); J. Li, and K. Chang, Appl. Phys. Lett. 95, 222110 (2009).
[21] O. P. Sushkov, and A. H. Castro Neto, Phys. Rev. Lett. 110, 186601 (2013).
[22] M. S. Miao, Q. Yan, C. G. Van de Walle, W. K. Lou, L. L. Li, and K. Chang, Phys. Rev. Lett. 109, 186803 (2012).
[23] R. Pillarsetty, Nature 479, 324-328 (2011).
[24] V. F. Mitin, et al., Phys. Rev. B 84, 125316 (2011).
[25] M. K. Hudait, et al., J. Vac. Sci. Technol. B 051205 (2012).
[26] Y. Huo, et al., Appl. Phys. Lett. 98, 011111 (2011).
[27] S. J. Wojtczuk, et al. IEEE Trans. Electron. Dev. 37, 455 (1990).
[28] G. -L. Luo, et al. J. Electrochem. Soc. 157, H27 (2010).
[29] A. Christou, W. T. Anderson, Jr., J. E. Davey, M. L. Bark, and Y. Anand, Electron. Lett. 16, 254-256 (1980).
[30] V. F. Mitin, V. V. Kholevchuk, B. P. Kolodych, Cryogenics 51, 68 (2011).
[31] V. F. Mitin, Yu A. Tkhorik, and E. F. Venger, Microelectronics J., 28, 617-625 (1997).
[32] P. E. Blöchl, Phys. Rev. B 50, 17953 (1994).
[33] G. Kresse and J. Furthmuller, Phys. Rev. B 54, 11169 (1996).
[34] J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. 118, 8207-8215 (2003).
[35] J. E. Peralta, J. Heyd, G. E. Scuseria, and R. L. Martin, Phys. Rev. B 74, 073101 (2006).
[36] M. Cardona, N. E. Christensen, and G. Fasol, Phys. Rev. B 38, 1806 (1988).
[37] S. Richard, F. Aniel, and G. Fishman, Phys. Rev. B 70, 235204 (2004).
[38] M. El Kurdi, S. Sauvage, G. Fishman, and P. Boucaud, Phys. Rev. B 73, 195327 (2006).
[39] P. O. Löwdin, J. Chem. Phys. 19, 1396 (1951).
[40] See on-line supplemental material at [URL will be inserted by publisher] for details of 30-band \mathbf{k}\cdot\mathbf{p} theory.