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Piezotronic Transistor Based on Topological Insulators

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ABSTRACT: Piezotronics and piezophototronics are emerging fields by coupling piezoelectric, semiconductor and photon excitation effects for achieving high-performance strain-gated sensors, LEDs, and solar cells. The built-in piezoelectric potential effectively controls carrier transport characteristics in piezoelectric semiconductor materials, such as ZnO, GaN, InN, CdS and monolayer MoS_2. In this paper, a topological insulator piezotronic transistor is investigated theoretically based on HgTe/CdTe quantum well. The conductance, ON/OFF ratio, and density of states have been studied at various strains for the topological insulator piezotronic transistor. The ON/OFF ratio of conductance can reach up to 10^{10} with applied strain. The properties of topological insulator are modulated by piezoelectric potential, which is the result of piezotronic effect on quantum states. The principle provides a method for developing high-performance piezotronic devices based on topological insulator.

Piezoelectric semiconductors have the coupling properties of piezoelectric and semiconductor, such as ZnO, GaN, InN and CdS. The emerging fields of piezotronic and piezophototronic have attracted much attention for flexible energy harvesting and sensor applications.[1, 2] A series of multifunctional electromechanical devices have been developed by nanostructure piezoelectric semiconductor, such as nanogenerator,[3-5] piezoelectric field effect transistor,[6] high-sensitivity strain sensor,[7] piezo-phototronic photocell,[8] and LED.[9] Piezotronic logic devices based on strain-gated transistors can convert mechanical stimulus to digital signal for logical computation.[10-12] Taxel-addressable matrices[13] and photon-strain sensor arrays[14] have been fabricated for integrated chips. Furthermore, nanogenerator and piezotronic transistor have been developed by single-atomic-layer MoS_2.[15, 16]

For high sensitivity of piezotronic and piezophototronic devices, strain-induced piezoelectric potential plays a key role by controlling carrier generation, transport, and recombination.[17-19] The width of piezoelectric charge distribution is an important parameter for improving performance of piezotronic transistor. By using the density functional theory, our previous theoretical studies have calculated the width of piezoelectric charge distribution in piezotronic transistors based on different metal and semiconductor.[20, 21] Furthermore, piezoelectric charges change wavelength and enhance luminescence in quantum devices, such as ZnO nanowire, single-atomic-layer MoS_2 and CdTe quantum dot devices.[22-25]

Topological insulators have been revealed theoretically and experimentally based on HgTe/CdTe quantum well structure,[26-28] which have potential application for low energy consumption and quantum computer.[29, 30] The static strain can create or destroy topological insulator states, such as HgTe and Bi_2Se_3 topological insulator.[31, 32] Recent theoretical results present that the coupling of strong electric field and strain can create topological insulator states in GaN/InN/GaN quantum well.[33]

In this paper, topological insulator piezotronic transistor is proposed based on HgTe/CdTe quantum well structure. A thin HgTe layer is sandwiched between two CdTe layers to form a quantum well which has an inverted band. Strain-induced piezoelectric field modulates the electron transport in HgTe quantum wells. Therefore, the piezotronic transistor based on topological insulator is a mechanically manipulating device using by the piezotronic effect. The ON/OFF conductance ratio can reach up to 10^{10}. Piezotronic transistor based on topological insulator can be used for high performance and ultra-low power consumption switch, logical unit and strain sensor.

To illustrate the piezotronic transistor based on topological insulator, Figure 1 shows the HgTe/CdTe quantum well structure with split gate on the side of HgTe. The constriction between the left and right gate acts as quantum point contact (QPC).[34] The width of quantum point contact can be turned by piezoelectric potential. Figure.1 (a) shows a gapless band structure in quantum point contact without piezoelectric potential, which is typical topological insulator based on the HgTe/CdTe quantum well structure. The current can flow across quantum point contact region without piezoelectric potential. This state is “ON” state of this device. The width of quantum point contact decreases while the piezoelectric potential increases. While the band gap is formed by applied strain, the conducting channel closes, as shown in Figure.1 (b). Therefore the electrons will be blocked and reflected back, resulting in “OFF” state.

Piezotronic transistor based on topological insulator is a quantum piezotronic device, which uses piezoelectric field to control the conductance of topological insulator. Initial state is topological insulator state without applied strain. Energy band structure of topological insulator state changes from gapless to having a gap by applying strain. In the case of HgTe/CdTe quantum well structure, strain-induced piezoelectric field is parallel to the surface of topological insulator. The direction of piezoelectric field also can be perpendicular to surface of topological insulator. For example, in case of GaN/InN/GaN quantum well structure, the band gap becomes smaller while the strain-induced piezoelectric field increases.[33] Thus, topological insulator states are formed by strain-induced piezoelectric field.

Besides above two type topological insulator based piezotronic transistor, possible structures of using piezoelectric field to control topological insulator states are GaAs/Ge/GaAs quantum well [35] and two-dimensional transition metal dichalcogenides [36], such as MoS_2, $MoSe_2$ and WSe_2.

Electronic transport in the quantum well can be described by Schrödinger equation

$$H\psi = E\psi \tag{1}$$

where H is Hamiltonian, ψ is wave function and E is eigenvalue. By solving Schrödinger equation under the boundary condition, the wave function can be obtained to calculate the transport properties, including the density of states (DOS), the transmission and the conductance.

Take a typical HgTe/CdTe quantum well topological insulator as example, electronic properties are described by the four-band Hamiltonian of the Bernevig-Hughes-Zhang (BHZ) model[26]

$$H(k)=\begin{bmatrix} \varepsilon_k+M_k & Ak_- & 0 & 0 \\ Ak_+ & \varepsilon_k-M_k & 0 & 0 \\ 0 & 0 & \varepsilon_k+M_k & -Ak_+ \\ 0 & 0 & -Ak_- & \varepsilon_k-M_k \end{bmatrix} \tag{2}$$

where $k=(k_x,k_y)$ is the in-plane momentum of electrons, $\varepsilon_k=C+V(x)-Dk^2$, $M_k=M-Bk^2$, $k_\pm=k_x\pm ik_y$ and $k^2=k_x^2+k_y^2$, $V(x)$ is the confinement potential of quantum well. A,B,C,D,M are the expansion parameters describing the band structure of HgTe/CdTe quantum well. The topological property of the HgTe/CdTe quantum well depends on the thickness of HgTe layer which has the critical values d_c.[26] While the thickness is less than the critical thickness d_c, the quantum well is the normal insulator state. The thickness is larger than d_c, the band energy of quantum well is the topological insulator state. In this study, the thickness of HgTe is set at 7nm ($>d_c=6.3$ nm), a typical value for topological insulator state of the device. The material parameters used in this study are $A=364.5$ meV nm, $B=-686$ meV nm^2, $C=0$, $D=-512$ meV nm^2 and $M=-10$ meV.[26]

The conductance is given from Landauer-Büttiker formula[37, 38]

$$G=G_0\sum_{m,n}\left|t_{nm}\right|^2 \tag{3}$$

where t_{nm} is the transmission coefficient for electron from the n-th input mode to the m-th output mode, G_0 is the conductance quantum which is defined as e^2/h.

For a small uniform mechanical strain *S*, the polarization vector *P* is given by[39]

$$(\mathbf{P})_i = (\mathbf{e})_{ijk}(\mathbf{S})_{jk} \tag{4}$$

where e_{ijk} the third order tensor is the piezoelectric tensor.

According to piezoelectric theory, the constituter equations can be given by[17, 40]

$$\begin{cases} \boldsymbol{\sigma} = \mathbf{c_E S} - \mathbf{e^T E} \\ \mathbf{D} = \mathbf{eS} + \mathbf{kE} \end{cases} \tag{5}$$

where $\boldsymbol{\sigma}$, $\mathbf{c_E}$ are the stress and elasticity tensor, $\mathbf{E}$ and $\mathbf{D}$ are the electric field and displacement, and $\mathbf{k}$ is the dielectric tensor.

Thus, piezoelectric potential induced by applied strain can be obtained as

$$V_{piezo} = \frac{PL_{piezo}}{\varepsilon_r \varepsilon_0} \tag{6}$$

where L_{piezo} is the length of piezoelectric material, ε_r is the relative dielectric constant and ε_0 is the vacuum dielectric constant.

Considering zinc-blende structure CdTe grown along [111] direction[41] with shear strain s_{23} of y-z plane, the piezoelectric potential is given by

$$V_{piezo} = \frac{e_{14} s_{23} L_{CdTe}}{\varepsilon_r \varepsilon_0} \tag{7}$$

where e_{14} is the piezoelectric coefficient of CdTe, L_{CdTe} is the length of CdTe in topological insulator.

For wurtzite structure GaN[42] with strain s_{11}, s_{22}, s_{33} along x, y, z direction, the piezoelectric potential can be given by

$$V_{piezo} = \frac{\left(e_{33}s_{33} + e_{31}s_{11} + e_{31}s_{22}\right) L_{GaN}}{\varepsilon_r \varepsilon_0} \tag{8}$$

where L_{GaN} is the length of GaN in topological insulator.

RESULTS AND DISCUSSION

Piezotronic Transistor Based on Topological Insulator. Figure 2(a) shows a schematic of the strain modulation of electron transport in quantum well. The strain-induced piezoelectric potential is applied on the left and right gate which is located on the top of HgTe/CdTe quantum well.[43] The split gate can affect the extension of the depletion regions of quantum well,[44] which can restrict electrons travelling through the system. In HgTe/CdTe quantum well structure topological insulator based piezotronic devices, the split gate voltage is supplied by piezoelectric potential and bias voltage.

For wurtzite structure GaN/InN/GaN quantum well, tensile and compressive strain can induce piezoelectric charges in the interface and a perpendicular piezoelectric field is created in the quantum well. The piezoelectric field will change normal insulator state to topological insulator state in GaN/InN/GaN quantum well.

HgTe/CdTe quantum well is a good candidate of topological insulator for quantum piezotronic device. The substrate of HgTe/CdTe quantum well can be designed by zinc-blende structure piezoelectric semiconductors, such as GaAs, GaP, InSb and InAs. According to the piezoelectric equation, the polarization charges can be obtained from (4) and (5). The piezoelectric coefficient e_{14} and relative dielectric constant ε_s are listed in TABLE 1.[45]

In case of piezoelectric field parallel to the surface of topological insulator, the width of the QPC can be effectively controlled by applied strain on piezoelectric semiconductor. Previous experiments presented that the width of the QPC W_{QPC} is approximately linear dependence on the split-gate voltage.[46] Therefore, W_{QPC} is proportional to piezoelectric potential in QPC region, which is given by

$$W_{QPC} = \alpha\left(V_{piezo} + V_0\right) + W_0 . \tag{7}$$

where α is the parameter depending on topological insulator material and device structure. V_0 is the bias voltage between left and right gate, W_0 is the width of the QPC without piezoelectric potential. The parameters used in the calculation are $\alpha = 225$ nm V^{-1}, $V_0 = 0.87$ V and $W_0 = 300$ nm.[46]

The piezoelectric potential is a linear function of shear strain s_{23} with different piezoeletric semiconductors, as shown in Figure 2(b). The piezoelectric potential increases with applied strain for CdTe. Due to the opposite sign of the piezoelectric coefficient, the piezoelectric potential decreases with strain for GaAs, GaP, InSb and InAs. Figure 2(c) shows the width of the QPC at various strain from -2.0 % to 2.0 %.

In our simulation, the Fermi energy is $E_F = 10$ meV. At this condition, the system has one topological edge channel. Figure 2(d) shows that the conductance G changes with external strain s_{23}. The conductance changes from “ON” to “OFF” state at strain of -1.5% in case of CdTe. While applied strain is larger than switching point, the band gap E_g appears. As a result, the electrons are blocked. In addition, the energy band shows gapless structure of topological insulator while applied strain is less than switching point. For GaAs, GaP, InSb and InAs, the strain switching point is 0.36%, 0.54%, 1.21% and 1.75%, respectively. Thus, the conductance can be effectively controlled by strain. This is the piezotronic effect on topological insulator. The ON/OFF ratio of the conductance is up to 10^{10}. Therefore, the strain-gated piezotronic transistor offers a high performance and low power consumption strain-gated switch, which can be acted as strain-gated logical unit.

A design of topological insulator piezotronic switch is shown in Figure 3(a). The piezoelectric potential and bias voltage are applied to the gate. The strain applied on the piezoelectric semiconductor CdTe is plotted as a function of time in Figure 3(b). The strain varies from -1.6% to -1.0%. The conductance changes from near zero to $2G_0$, corresponding to “OFF” and “ON” state, respectively.

The sensitivity of piezotronic strain sensor can be calculated by

$$R = \frac{d\left(G/G_0\right)}{ds_{23}}. \tag{8}$$

The maximum values of sensitivity and corresponding strain are shown in Figure 3(c). It clearly shows that the maximum sensitivity is larger than 10^3, For GaAs and GaP, the maximum value of sensitivity can reach over 10^4. Figure 3(d) shows switch and strain sensor region divided by the sensitivity. The amplitude of the sensitivity show sharply changes at sensor region.

Piezotronic Effect on Surface-States of Topological Insulator. Topological insulators based on HgTe quantum well structure have gapless surface states and an insulating bulk. Figure 4(a) shows the conductance of topological insulator surface as a function of strain. The Fermi energy is fixed at $E_F = -15$ meV. The local densities of states (LDOS) of spin-down electrons for “OFF” and “ON” states are shown in Figure 4(b) and (c), respectively. In our simulation, the calculated widths of the QPC are $W_{QPC} = 40$ nm and 10 nm, corresponding to strain of -1.67% and -1.78%, respectively. The spin-up properties can also be obtained by KWANT software package.[47] The surface states of topological insulators present strain-modulated transport properties using by strain-induced piezoelectric field.

Previous theoretical results presented that the more conducting channels from bulk states can be created while the Fermi energy increases.[34, 48] There are three channels: one is edge channel and two are bulk channel, as shown in Figure 4(a). Three conductance plateaus can be created while the strain changes. Each conducting channel contributes a conductance ($2e^2 / h$) to the total conductance. In case of HgTe/CdTe quantum well, the edge channel in the QPC is created while the strain changes from -1.74% to -1.48%. While the strain increases from -1.32% to -1.17%, the width of the QPC increases. One bulk channel in the QPC is formed, which contributes a conductance plateau to double the total conductance. This is the mechanism of the second conductance plateau. While the strain increases from -0.92% to 0, the third conductance plateau appears. The conductance steps are plotted for GaAs, GaP, InSb and InAs, as shown in Figure 4(a).

CONCLUSIONS

In this study, we have proposed a strain modulation of electronic transport in topological insulator. Two type piezotronic transistors have been demonstrated based on topological insulator of HgTe/CdTe and GaN/InN/GaN structure, corresponding to normal open and normal close switch, respectively. The strain-induced piezoelectric potential is used to control the width of the QPC, and affects electronic transport of piezotronic transistor based on topological insulator. A transition is shown when conductance changes from near zero to the conductance, which presents high ON/OFF ratio of 10^{10}. Piezotronic logical unit and high sensitivity strain sensor can be designed by the strain-gated piezotronic switch. Furthermore, the multiple conductance steps for higher Fermi energy are investigated at various strains. This study provides not only the guidance for developing high-performance piezotronic spin devices, but also a theoretical insight of using piezotronic effect on physical properties of spin transport.

METHODS

The conductance of this quantum spin Hall system is calculated by KWANT code. KWANT is free software and has obtained wide application in the numerical calculation of quantum transport in nanostructure system. KWANT solves the scattering problem by using the wave-function approach.

FIGURES

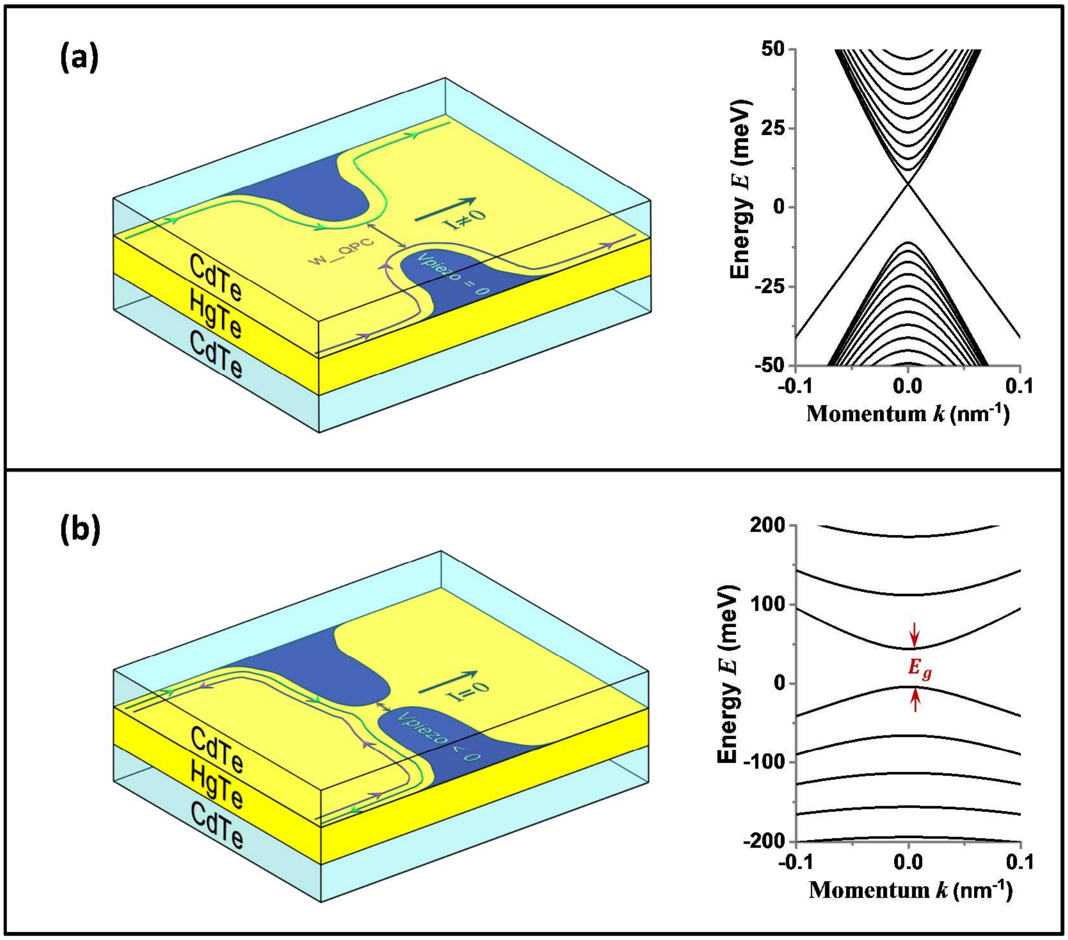

Figure 1. Schematics of electronic transport and energy band controlled by the QPC in the HgTe/CdTe topological insulator. The spin-up (green line) and spin-down (purple line) electrons travel along boundary. (a) gapless Dirac cone for the wide QPC, and (b) energy gap E_g emerging for the narrow QPC.

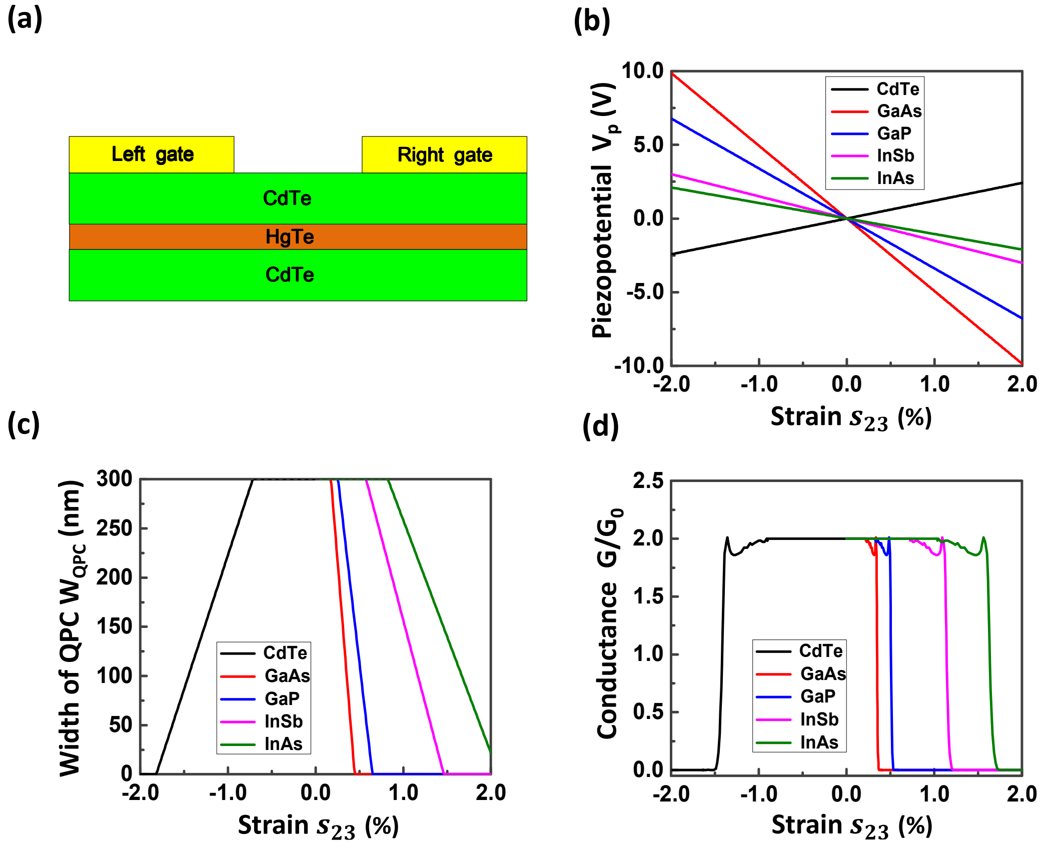

Figure 2. (a) Schematic of controlling the width of the QPC by left and right gate voltage on the top CdTe layer. (b) The piezoelectric potential as a function of strain under different piezoelectric semiconductor materials (CdTe, GaAs, GaP, InSb and InAs). (c) The width of the QPC as a function of strain. (d) The conductance as a function of strain at fixed Fermi energy $E_F = 10$ meV.

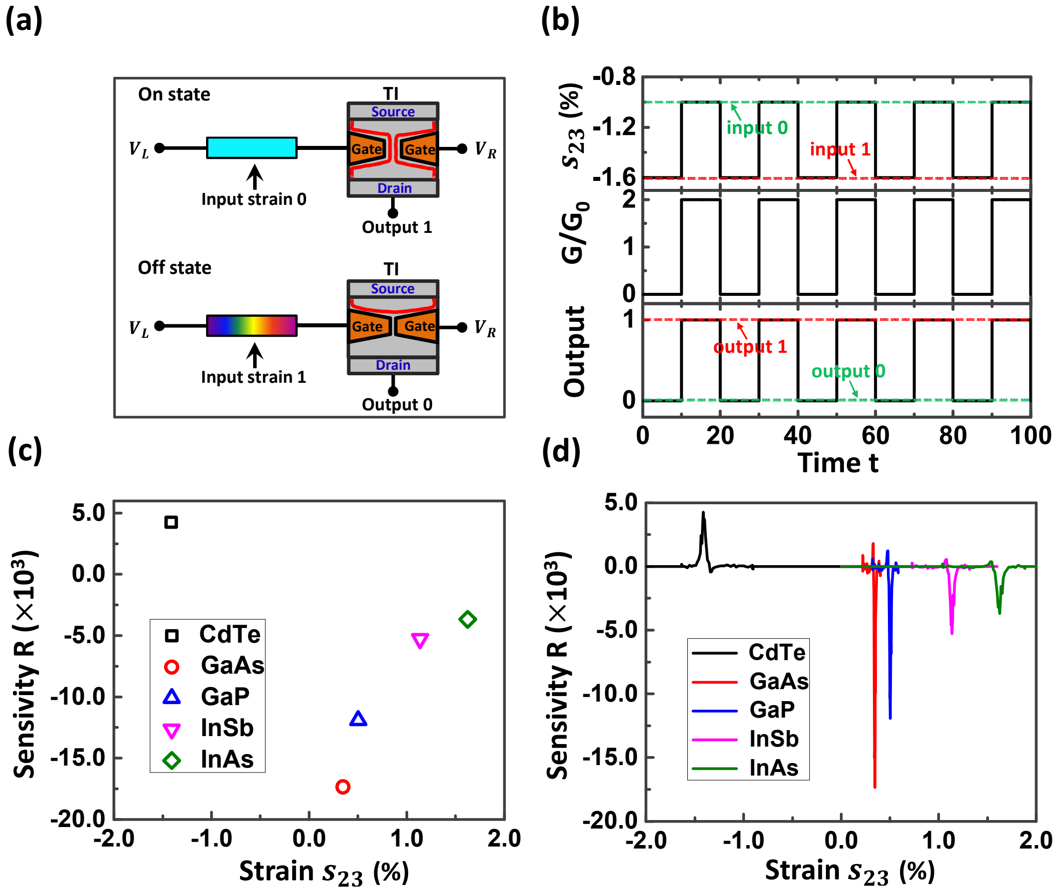

Figure 3. (a) Schematic of piezotronic switch based on topological insulator. The output signal 1 is "ON" state and 0 is "OFF" state. (b) The applied strain, conductance, and output signals change with time. (c) The maximum value of sensitivity for different piezoelectric semiconductor materials. (d) The sensitivity *versus* strain.

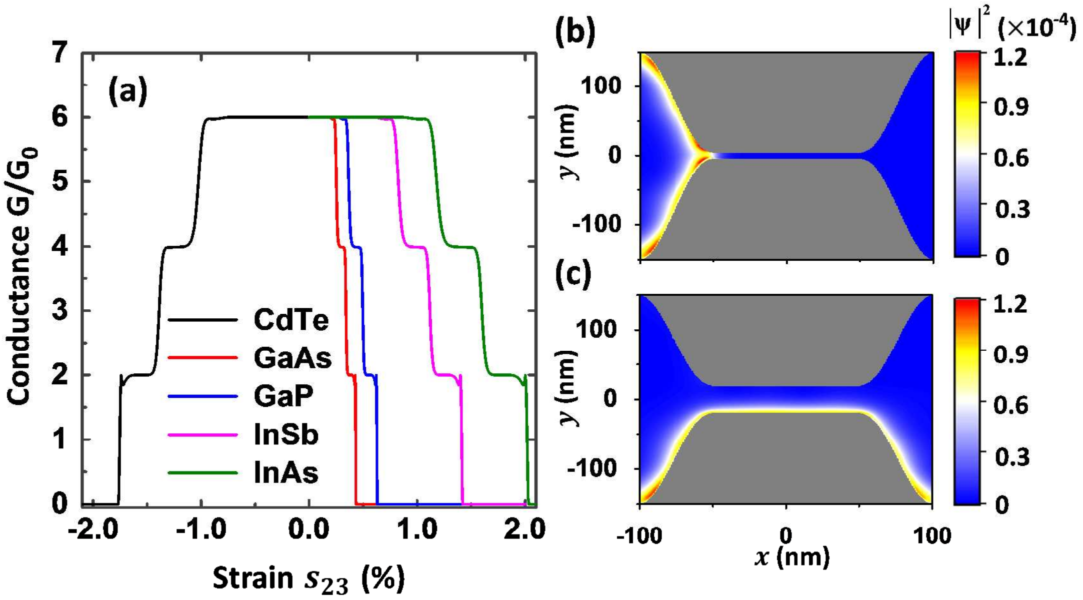

Figure 4. The conductance as a function of strain for different piezoelectric materials, the Fermi energy is fixed at $E_F = -15\,\text{meV}$. Wave function of spin down electrons (edge states) (b) OFF state at $W_{QPC} = 10\,\text{nm}$, and (c) ON state at $W_{QPC} = 40\,\text{nm}$.

Table 1. Piezoelectric Coefficient and Relative Dielectric Constant for the Crystals of Cubic Symmetry

material	piezoelectric coefficient e_{14} (C/m^2)	relative dielectric constant ε_r	reference
CdTe	0.035	9.8	[41]
GaAs	-0.16	11	[45]
GaP	-0.1	10	[45]
InSb	-0.071	16	[45]
InAs	-0.045	14.5	[45]

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G.H. and Y.Z. contributed equally to this work. G.H., Y.Z and Z. L.W. designed the system, G.H. and Y.Z. performed the calculations, analyzed the data, and wrote the paper. L.L. analyzed the data. Z. L.W. supervised the study, analyzed the data, and revised the paper.

Notes

The authors declare no competing financial interest.

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