Tuning Spin Hall Conductivity in GeTe by Ferroelectric Polarization

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Controlling charge-spin current conversion by electric fields is crucial in spintronic devices, which can now be realized in diatom ferroelectric semiconductor GeTe. It is well demonstrated that ferroelectricity can change the spin texture in this compound. Herein, it is shown that the spin Hall conductivity (SHC) can be further tuned by ferroelectricity based on the density functional theory calculations. The spin texture variation driven by the electric fields is elucidated from the symmetry point of view, highlighting the interlocked spin and orbital degrees of freedom. It is observed that the origin of SHC can be attributed to the Rashba effect and the intrinsic spin–orbit coupling. The magnitude of one component of SHC $\sigma_{xy}$ can reach as large as $100 \, \hbar/e \, (\Omega^{-1} \, \text{cm}^{-1})$ in the vicinity of the band edge, which promises engineering spintronic devices. The work on tunable spin transport properties via the ferroelectric polarization brings novel assets into the field of spintronics.

1. Introduction

Spintronics is a multidisciplinary subject where the coupling of spin and orbital degrees of freedom of electrons plays an important role. The most important consequence of this coupling is the conversion of charge current into a spin current, which is called spin Hall effects (SHEs). This interconversion has been found in many different materials, such as heavy metals, semiconductors, and interfaces between oxides, for example, LaAlO$_3$/SrTiO$_3$ (LAO/STO). Manipulation of the charge–spin conversion is one of the keys to successful applications of spintronic devices. The controllable spin–orbit coupling (SOC) leading to a gateable electric signal in LAO/STO was recently shown by several groups, as reviewed by Han et al. The underlying mechanism is the change of the electron density which changes the occupation of different orbitals. Tsymbal and co-workers discovered tunneling anomalous Hall effect (TAHE) in a ferroelectric tunnel junction, where the ferroelectric barrier endowed with tunable Rashba SOC. In the work by Matos-Abiague and Fabian, the Rashba SOC at the interfacial between the ferromagnetic metal and the normal semiconductor results in a spin-dependent momentum filtering can also induce TAHE and SHEs. Very recently, another material family was proposed to show electrically controllable spin–orbit coupling based on ferroelectricity, called ferroelectric Rashba semiconductors (FERSO). These materials are GeTe, SnTe, and MX$_2$. Among them, GeTe, a narrow gap semiconductor, received special interests due to its wide range of properties for modern functional materials such as thermoelectricity, ferroelectricity, or electrical phase change within such simple stoichiometry and the two-atom rhombohedral unit cell. Both experiments and theoretical calculations show that the Rashba coupling strength in GeTe can be tuned by the electric polarization; meanwhile, the spin texture is also related to the electric polarization as shown by theoretical calculations and spin-resolved angular resolved photoemission spectroscopy (ARPES). Both results show that the clockwise winding directions in the reciprocal space of the spin vectors can be reversed to anticlockwise. Very recently, Wang et al. calculated the spin Hall conductivity (SH) of GeTe and SnTe in the ferroelectric and paraelectric states. The ferroelectricity can be sustained even in the hole-doped phase. The SHE can be achieved in a polar phase. There are several other ferroelectric compounds which show the reversible spin texture controlled by electric polarization, such as HfO$_2$, KTaO$_3$, BiAlO$_3$, BiInO$_3$, PbTiO$_3$, BiTeI, and GeTe/InP superlattice. The controllable spin texture may lead to control of the spin precession, so that the proposal of spin transistor may be realized, as in the recently demonstrated ferromagnetic-free all-electric spin Hall transistor. Although the spin texture can be tuned by the polarization as clearly shown by the ARPES, it is still not shown how the spin current to charge current conversion is influenced. This conversion is the crucial step to utilize the effect in real devices. The spin-to-charge conversion in GeTe was observed by Rinaldi et al. for the first time.
time. However, the tuning of the conversion efficiency was not reported yet.

In this work, we show by ab initio calculations, as well as by general argument based on the effect of electric polarization on the spin texture, that the electric field can be used to tune the SHC which is contributed from both the Rashba effect due to polarization and the bulk effect. The former one is only marginally influenced, whereas the latter effect near the band edge is enhanced obviously under ferroelectric distortions and even the sign can be changed. It is thus possible to tune the magnitude of the SHC.

In the following, we first outline the theoretical background and calculation details of the electronic structure and SHC in Section 2. Then, we argue that the dependence of the spin winding and the electric polarization is equivalent to switching of the coordinate system in Section 3.1 by the electronic band structure. We show the electric field dependence of the Rashba parameters in Section 3.2, and finally we show the polarization-dependent SHC in Section 3.3.

2. Calculation Details

GeTe crystallizes into the noncentrosymmetric rhombohedral structure (space group R3m, no. 160) with the rhombohedral lattice constant \(a = 4.373 \, \text{Å}\) and the angle \(\alpha\) between the axis 57.76°. Ferroelectric polarization is realized by the relative displacement of Ge and Te along the [111]-direction which is chosen as the z-axis in our calculations. The lattice parameters are fully relaxed when the polarization is changed. The electronic structure was calculated by the pseudopotential plane wave method (PWscf)\(^{[30]}\) within the generalized gradient approximation (GGA) parameterized by Perdew et al.\(^{[31]}\) The energy cut-off was set to 30 Ry and the Brillouin zone (BZ) integration was performed on a uniform grid with 20 \(\times\) 20 \(\times\) 20 \(k\)-points. The atomic positions are relaxed under a homogenous electric field using the theory developed by Nunes and Gonze,\(^{[32]}\) where the polarization is calculated by the modern theory of polarization. The force convergence criterion is set to 0.001 a.u. The electronic structure analysis was conducted by the graphic interface Virtual NanoLab (VNL).\(^{[33]}\) The Hilbert space with the plane wave basis was projected onto the maximally localized Wannier orbital spaces spanned the valence s- and p-orbitals. Calculations of the SHC were performed by the code developed by one of the authors,\(^{[34]}\) which evaluates the Kubo formula within the linear response theory. The intrinsic SHC can be obtained with the help of the concept of Berry curvature,\(^{[35]}\) which has the following form

\[
\sigma_{\alpha ij}^D = \frac{\hbar}{2 \pi} \sum_{\mathbf{k}} \int_{\mathbf{BZ}} \frac{d^2 \mathbf{k}}{(2\pi)^2} f_n(\mathbf{k}) \Omega^D_{\alpha ij}(\mathbf{k})
\]

where \(\Omega^D_{\alpha ij}(\mathbf{k})\) is referred as the spin Berry curvature defined as

\[
\Omega^D_{\alpha ij}(\mathbf{k}) = 2i \hbar^2 \sum_{\mathbf{m}, \mathbf{n}} \langle u_{\mathbf{n}}(\mathbf{k}) | \{ \bar{v}_{\mathbf{n}} | u_{\mathbf{m}}(\mathbf{k}) \} \rangle \langle \bar{v}_{\mathbf{n}} | u_{\mathbf{m}}(\mathbf{k}) \rangle \langle u_{\mathbf{n}}(\mathbf{k}) | \bar{v}_{\mathbf{m}}(\mathbf{k}) \rangle
\]

with \(\alpha, \beta, \gamma = x, y, z\) and \(m, n\) being the band indices. The spin current operator is \(j_\gamma = \frac{1}{2} \{ \bar{v}_\gamma, \bar{\sigma}_\gamma \}\), where \(\bar{\sigma}_\gamma\) is the spin operator component \(\gamma\) and \(\bar{v}_\gamma\) is the velocity operator component \(\alpha\). The Fermi Dirac distribution function \(f_n(\mathbf{k})\) is the mean occupation number of states labeled by \((n, \mathbf{k})\) at a finite temperature \(T\). In this work, we set \(T = 0\, \text{K}\). The third-order tensor \(\sigma_{ij}^D\) represents the spin current \(j_\gamma^D\) generated by an electric field \(\mathbf{D}\) via \(j_\gamma^D = \sigma_{ij|\gamma}^D D_j\). The spin current is polarized in the \(\gamma\)-direction and flows in the \(\alpha\)-direction, for an electric field applied in the \(\beta\)-direction.

The integral over the \(k\)-space during the calculation of the SHC was sampled in the first BZ with grids of \(200 \times 200 \times 200\) to ensure the convergence. The unit of SHC is \(\hbar / e \, (\Omega^{-1} \text{ cm}^{-1})\).

3. Results and Discussion

3.1. Electronic Structure and Ferroelectricity

The Kohn–Sham band structure calculated using the experimental lattice constants is shown in Figure 1, where a comparison of the results with and without the SOC is also made. Without the SOC, the ferroelectric distortion leads to the direct bandgap of about 0.66 eV near the L-point as shown by the dashed blue curves. The value is only 0.05 eV higher than the experimental value reported by Park et al.\(^{[36]}\) We noted that even in the absence of SOC, there are humps around the L-point due to the electric polarization. The SOC leads to splitting (\(\Delta_{\text{SOC}}\)) of the bands about 0.7 eV along the \(\Gamma-L\) line, which indicates that the SOC field is more or less unidirectional. However, the Rashba-like splitting is only around the L-point, and obvious at the valence band maximum (VBM) at L as shown by the solid green lines. This direction in our coordinate system is in the direction of polarization. The contributions of the SOC are mainly observed in the valence bands because they are mostly from the Te 5p orbitals, whereas the conduction bands are from the Ge 2p orbitals. This is in contrast to a simple interpretation of resonant bonds because the 5p states of Te are much higher in energy than the 2p states of Ge.

Figure 1. Comparison of the Kohn–Sham band of GeTe without (dashed blue curves) and with SOC (solid green curves). The vertical double arrow indicates the SOC splitting of the state \(\Delta_{\text{SOC}}\) along the \(\Lambda\)-line. The inset shows the path and the special \(k\)-points in the Brillouin Zone used in the calculations.
states of Ge. The so-called “cross gap hybridization” was used to depict this phenomenon in the highly ionic compound.\textsuperscript{37,38} This anomaly is related to the enhanced Born effective charge which in turn improves the bonding with distortion.

The band colored by the different spin components is shown in Figure 2. The dispersions of the bands for reversed polarization, namely $+P$ and $-P$ are the same. This is understandable because the ferroelectric displacement and spin-z directions are the same. If the SOC was overlooked, the spin polarization would be independent of the crystal coordinates. In this case, the spins are unaltered upon electric polarization reversal. At the L-point, the spin vectors in the $X$ and $Y$ directions have different contributions when the $k$-path is along $L-U$ and $L-W$ directions, as shown in Figure 2a,c. These contributions are reversed when the polarization is reversed from $+P$ to $-P$. As a result, due to the SOC, the winding directions of the spin vectors are reversed in the $k$-space as reported in previous works.\textsuperscript{11} We noted that there is no $x$ nor $y$-components contributions along $\Gamma-L$ which indicates a unidirectional SOC field along this path as shown by the almost rigid shift $\Delta_{SOC}$ due to SOC field in Figure 1. At the same time, we plotted the $z$-component of the spin in Figure 2b,d. It can be seen that the different polarization also changes the projection weight. The changing of the spin winding direction can be understood as following: in real space, the polarization reversal is equivalent to change the $z$-component of the coordinate system. In this case, the $x$-$y$ axis changes from the right-handed to the left-handed as the viewpoints are changed from the z to $-z$-axis. This effect is universal in ferroelectric materials\textsuperscript{22,23,25–27} as it is related to the changing of the coordinate system once the polarization reversal is realized only by the relative shift of the atomic positions. This effect can also be clearly seen from the electron isosurface of the different spin components as in Figure 3. In this figure, we show the negative polarization in a cell that is rotated upside down so that the atomic positions are the same as shown in Figure 3a,b. As observed from the figures, in this case, the spin densities of $x$, $y$, and $z$-components are the same, so that the spin moment direction is the same. However, the $z$-axis of the coordinates is reversed, which gives the polarization direction. In this way, the spin directions are interlocked with the ferroelectric polarization.

3.2. Spontaneous Polarization and Rashba Coupling

The ferroelectricity in GeTe was well explored and understood more than 50 years ago.\textsuperscript{39,40} The soft optical phonon is the cause of the displacive movement of the diatomic compound. In GeTe, ferroelectric displacement of Te along [111] shows double-well energy minimums at $\tau = 0.03 \ a_0$ away from the middle point.
of the diagonal. The potential barrier height is about 54 meV, which is double as that of BaTiO$_3$ and half as that of PbTiO$_3$.\cite{41} This indicates that the Curie temperature about 670 K of GeTe lies between them. The spontaneous ferroelectric polarization of 67 $\mu$C cm$^{-2}$ was obtained by the Berry phase theory of polarization. The Born effective charge ($Z^*$) was estimated by the finite difference method from the expression\cite{30}

$$\delta P = \frac{e}{\Omega} Z^* \cdot \delta u$$

where $\delta u$ is the first-order change of the positions of Te and $\Omega$ is the volume of the unit cell. We estimate the $Z^*$ being about 9.58 e using the data where $u$ is below 0.1 Å. This is a value at the same scale of other usual ferroelectric compounds indicating the strong interactions of the orbitals between Te and Ge along the [111]-direction.

Electric field is an effective way to tune the properties of ferroelectric materials. Due to the polarization, the electric field induces displacements of the ions and the electronic structure changes accordingly as shown in Figure 4. The nonlinearity and asymmetry is apparent when the electric field gets larger in the two different directions. The Zener breakdown field $E_{zb}$ is estimated to be $E_{zb} = E_g / L \sim 0.01$ a.u. = 51 MV cm$^{-1}$, where $E_g$ is the bandgap and $L$ is the length of the unit cell in the direction of the electric field. In our calculations, the maximum field strength is about one order smaller than the breakdown field to avoid instability of the calculation. As expected when the field is along the direction of polarization, the Rashba splitting $E_R$ varies linearly with the electric field ($\vec{E}$) as understood by the Bychkov–Rashba Hamiltonian\cite{42}

$$H_R = \alpha_R \left( \vec{D} \right) \cdot \left( \vec{e}_z \times \vec{k} \right)$$

$$E_{RSO} = \frac{\hbar^2}{2m} \left( |k|| \pm k_R \right)^2 - E_R$$

where $\vec{k}$ = ($k_x$, $k_y$, 0) and $\vec{e}_z$ = (0, 0, 1). The nature of the phenomenon allows us to use the 2D electron gases (2DEG) model to get the related parameters. The spin degeneracy of the 2DEG is lifted and the energy dispersion has the form

3.3. SHC and its Dependence on the Ferroelectric Polarization

Because the intrinsic SHC is fully determined by the band structure, it is compatible with the symmetry of the Hamiltonian. We, therefore, figure out the nonzero matrix elements by symmetry analysis\cite{44} to simplify the computation of the third-order tensors.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{The electron isosurface of different spins with ferroelectric polarization a) $+P$ and b) $-P$. Note that in the two subfigures, the polarizations are plotted in the same directions, whereas the z-axis of coordinate system is turned upside down. The yellow, blue, and red denote the spin in the x, y, and z directions.}
\end{figure}
Due to the symmetry constraints, there are only four nonzero elements $\delta_i (i = 0, 1, 2, \text{and } 3)$. The full SHC tensors are listed as following

\[
\begin{align*}
\sigma_x: & \begin{pmatrix} \delta_0 & 0 & 0 \\ 0 & -\delta_0 & -\delta_1 \\ 0 & -\delta_2 & 0 \end{pmatrix}, & \sigma_y: & \begin{pmatrix} 0 & -\delta_0 & \delta_1 \\ -\delta_0 & 0 & 0 \\ \delta_2 & 0 & 0 \end{pmatrix}, \text{ and} \\
\sigma_z: & \begin{pmatrix} \delta_3 & 0 & 0 \\ 0 & -\delta_3 & 0 \\ 0 & 0 & 0 \end{pmatrix}
\end{align*}
\]

The nonzero elements calculated at the stationary state with ferroelectric polarization are shown in Figure 5. All the tensor components are of the same order of magnitude about $100 \, \hbar/e (\Omega^{-1} \text{ m}^{-1})$ around the conduction band minimum (CBM) and VBM. We see that there is much larger SHC amount to $900 \, \hbar/e (\Omega^{-1} \text{ cm}^{-1})$ around 2 eV below the VBM. When comparing with the band structure in Figure 1, we see that there is a large SOC shift ($\Delta_{\text{SOC}}$) of about 0.7 eV of the bands within this energy range. We may conclude that this large value comes from the large SOC-induced splitting of the band. Interestingly, the charge current $I$ and spin polarization $J_s$ are not necessarily perpendicular to each other. There are sizable contributions from $\delta_3$, namely $\sigma^{xy}_{\text{xx}}$ and $\sigma^{xy}_{\text{yx}}$, which means that we can get longitudinal spin Hall signal when the spin polarization is in-plane and perpendicular to the electric polarization. This value is peaked when the Fermi energy is about 1.1 eV above the CBM. This feature gives us more freedom to design spintronic devices when

![Figure 4](image-url)
optical pumping can be utilized. Recent preliminary experiments by Rinaldi et al.\(^{29}\) show that a charge current can be generated from the spin current. However, it is not clear whether it comes from the bulk or the interface. The SHC corresponding to the experimental setup is \(\sigma_{yz}\), which is \(\delta^2\) as shown in Figure 5. It is less than \(100 \hbar/e (\Omega^{-1} \text{cm}^{-1})\) according to our calculations and rather small compared with \(2200 \hbar/e (\Omega^{-1} \text{cm}^{-1})\) in Pt.\(^{45}\) At the same time, it is the same sign as Pt, which is not in agreement with the experiments. We may suggest that the experimental observations should not come from the bulk Rashba effect alone.

The maxima of \(\sigma_{yz}^2\) at the VBM and CBM are both about \(-100 \hbar/e (\Omega^{-1} \text{cm}^{-1})\) which are mainly due to the Rashba effect, in the sense that it is sensitively dependent on the electric polarization as shown in Figure 6, where the SHC is evaluated at several ferroelectric displacements (\(\tau\)). At the nonpolarized state, GeTe is metallic. Its SHC around the Fermi level is about \(100 \hbar/e (\Omega^{-1} \text{cm}^{-1})\). The value is peaked amount to \(110 \hbar/e (\Omega^{-1} \text{cm}^{-1})\) at 0.2 eV above the Fermi level. Even larger values can be obtained at the energy around \(-2.0 \text{ eV}\) below the Fermi level. We owe the SHC to the spin Berry curvature of the SOC band due to the equivalent SOC field because there is no Rashba effect. When the polarization is increased, we noted that the SHC around the CBM decreases, and even changes to the negative value. We may propose that the Rashba effect leads to negative SHC around the CBM and this value increases with the increase in the polarization. The increase in the SHC can be understood from the fact that the Rashba constant increases with the electric field, as shown already in Figure 4. As can be seen from Equation (2) and (5), \(\sigma_{yz}^2\) is an odd function of \(z\) and antisymmetric with respect to the interchange of \(x\) and \(y\). In this case, although the reversal of the polarization leads to the reversal of the spin vector winding, it does not lead to a sign reversal of the SHC tensor. We have numerically checked the SHC values when the polarization is reversed and find that it remains when the electric polarization is reversed.

4. Conclusions

To summarize, our theoretical calculation shows that the spin texture is closely related to the ferroelectric polarization. When the ferroelectric polarization is reversed, the spin winding direction is reversed accordingly. This is due to the change of the equivalent coordinate system upon the polarization reversal. It should be quite general in FERSC as shown in several compounds. The electric fields can tune the related Rashba parameters. The Rashba parameters increase with the electric field which naturally comes from its origin. The SHC is contributed from the intrinsic SOC and the Rashba effects, whereas the latter can be easily tuned by the external electric field. From the results, we suggest that the electric field can be utilized to moderate the spin and electron transportation properties of FERSC materials. It provides a new dimension to design spintronic devices.

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Conflict of Interest

The authors declare no conflict of interest.

Keywords

density functional theory calculations, ferroelectric semiconductors, spin Hall conductivity, spin–orbit coupling
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