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Spin Transport Properties of MnBi$_2$Te$_4$-Based Magnetic Tunnel Junctions

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The van der Waals heterojunctions, stacking of different two-dimensional materials, have opened unprecedented opportunities to explore new physics and device concepts. Here, combining the density functional theory with non-equilibrium Green’s function technique, we systematically investigate the spin-polarized transport properties of van der Waals magnetic tunnel junctions (MTJs), Cu/MnBi$_2$Te$_4$/MnBi$_2$Te$_4$/Cu and Cu/MnBi$_2$Te$_4$/h-BN/n-MnBi$_2$Te$_4$/Cu ($n = 1, 2, 3$). It is found that the maximum tunnel magnetoresistance of Cu/MnBi$_2$Te$_4$/h-BN/3-MnBi$_2$Te$_4$/Cu MTJs can reach 162.6%, exceeding the system with only a single layer MnBi$_2$Te$_4$. More interestingly, our results indicate that Cu/MnBi$_2$Te$_4$/h-BN/n-MnBi$_2$Te$_4$/Cu ($n = 2, 3$) MTJs can realize the switching function, while Cu/MnBi$_2$Te$_4$/h-BN/3-MnBi$_2$Te$_4$/Cu MTJs exhibit the negative differential resistance. The Cu/MnBi$_2$Te$_4$/h-BN/3-MnBi$_2$Te$_4$/Cu in the parallel state shows a spin injection efficiency of more than 83.3%. Our theoretical findings of the transport properties will shed light on the possible experimental studies of MnBi$_2$Te$_4$-based van der Waals magnetic tunnel junctions.

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The giant magnetoresistance and tunnel magnetoresistance (TMR) effects play important roles in the fields of information storage technology and designing of spintronic devices.\cite{1,2} Subsequently, the emergence of magnetic tunnel junctions (MTJs) prominently promoted the revolution of various spintronics.\cite{3–9} Compared with traditional electronic devices, the magnetic recording density of MTJs-based devices can be considerably enhanced, leading to the miniaturization of electronic devices. So far, much progress has been made, many problems and challenges still exist and need to be resolved for improvement of efficiency, performance, and stability of MTJs. For example, one of the research focuses is how to control the quality of the interface between the ferromagnetic layer and the barrier layer, because the interface influences the transmission of electrons with different orbital properties and unequal spin polarization. Therefore, the interface bonding has a profound effect on the conductance. Fortunately, the layered two-dimensional materials supported by van der Waals force without chemical bonding overcome these difficulties due to their advantages of layer-related thickness and ideal interface. Furthermore, constructing MTJs with two-dimensional materials also brings opportunities for exploring new physical phenomena and potential applications.\cite{10–17}

Since 2017, there has been great progress towards the development of two-dimensional (2D) magnetic materials. Numerous 2D materials have been synthesized experimentally,\cite{14–17} such as 2D ferromagnetic insulator CrI$_3$ and ferromagnetic metal Fe$_3$GeTe$_2$, providing abundant candidate materials to build MTJs. These 2D materials have been shown to be reliable platforms to construct high-performance MTJs through the layer-by-layer control of the thickness, sharp interfaces, and high perpendicular magnetic anisotropy. Compared with transition metal MTJs consisting of ferromagnetic electrodes and oxide barrier layers, it was reported that van der Waals MTJs by 2D magnetic layers exhibit superior performance.\cite{18–31} For instance, it was theoretically found that single/double-layered Fe$_3$GeTe$_2$-hBN-Fe$_3$GeTe$_2$ MTJs possessing prominent TMR effects, with the magnetoresistance ratio reaching up to 183% and 252%, respectively. When the Fe$_3$GeTe$_2$ MTJ is in the parallel state, a considerable spin polarization about 75% can be observed.\cite{21}

Later, layered MnBi$_2$Te$_4$ was successfully synthesized, and powder and single-crystal neutron diffraction measurements confirmed that the intra-and inter-layer magnetic orders are ferromagnetic and antiferromagnetic, respectively.\cite{32,33} As an intrinsic magnetic topological insulator, several exotic topological states have been proposed, e.g., quantized topological magnetoelectric effect and quantum anomalous Hall effect.\cite{32–35} Furthermore,
our previous study and the work of Zhan et al. on MnBi$_2$Te$_4$-based MTJs reported that giant TMRs as well as high spin polarization could be induced. However, in these studies, effect of the antiferromagnetic pinning layer on its transport properties was ignored. Therefore, it is necessary to explore the influence of the pinning layer on the MnBi$_2$Te$_4$-based MTJs.

In this work, we systematically investigate the spin current, spin injection efficiency (SIE), TMR and transmission coefficients of the Cu/MnBi$_2$Te$_4$/MnBi$_2$Te$_4$/Cu and Cu/MnBi$_2$Te$_4$/h-BN/n-MnBi$_2$Te$_4$/Cu (n = 1, 2, 3) MTJs by employing non-equilibrium Green’s function combined with the density-functional theory. In the presence of a pinning layer, we find that the maximum TMR of the Cu/MnBi$_2$Te$_4$/h-BN/3-MnBi$_2$Te$_4$/Cu MTJ can reach 162.6%, exceeding the system with only a single layer MnBi$_2$Te$_4$. More interestingly, our results indicate that Cu/MnBi$_2$Te$_4$/h-BN/n-MnBi$_2$Te$_4$/Cu (n = 2, 3) MTJs can realize the switching function, while the Cu/MnBi$_2$Te$_4$/h-BN/3-MnBi$_2$Te$_4$/Cu MTJ exhibits the negative differential resistance. Our findings demonstrate that the spin-related transport properties of these MnBi$_2$Te$_4$-based MTJs are highly dependent on the layer number and provide a promising platform for further experimental exploration of MTJs.

Fig. 1. Schematic of Cu/MnBi$_2$Te$_4$/MnBi$_2$Te$_4$/Cu, and Cu$_x$/MnBi$_2$Te$_4$/h-BN/n- MnBi$_2$Te$_4}$/Cu (n = 1, 2, 3). The red and blue arrows represent the magnetic orientation of Mn atoms in the parallel (P) state. The antiparallel (AP) magnetization structure can be obtained by reversing the magnetic direction of the free layer. These devices are periodic in the X and Y directions, and the current flows in the Z direction.

Model System and Theoretical Method. It is known that bilayer MnBi$_2$Te$_4$ is an insulator with A-type antiferromagnetic order. Figure S1 in the Supplementary Material shows the top and side views of the bilayer MnBi$_2$Te$_4$, respectively. Figures 1(a)–1(d) display our considered system structure of MnBi$_2$Te$_4$/h-BN/n-MnBi$_2$Te$_4$, where we utilize h-BN as the barrier layer and MnBi$_2$Te$_4$ as the ferromagnetic layer, respectively. The system is separated into three adjacent regions: the central scattering region, the left and right electrodes [i.e., Cu (111)], respectively. When constructing the central region, we consider four cases (ignoring the buffer layers), i.e., Cu/MnBi$_2$Te$_4$/MnBi$_2$Te$_4$/Cu, Cu/MnBi$_2$Te$_4$/h-BN/MnBi$_2$Te$_4$/Cu, Cu/MnBi$_2$Te$_4$/h-BN/2-MnBi$_2$Te$_4$/Cu, and Cu/MnBi$_2$Te$_4$/h-BN/3-MnBi$_2$Te$_4$/Cu MTJs.

Based on the nonequilibrium Green function combined with the density-functional theory, the spin-polarized current can be defined by the Landauer–Büttiker formula

\[
I_s = \frac{e}{h} \int T_s(E)(f_L(E) - f_R(E))dE,
\]

where \(\sigma = \uparrow, \downarrow\) denotes the index of spin, \(e\) is the electron charge, \(h\) is Planck’s constant, \(T_s(E)\) is the spin-resolved transmission coefficient, and \(f_{L(R)}(E)\) is the Fermi-Dirac distribution function of the left (right) electrode.

The TMR ratio with different bias voltages can be expressed as

\[
\text{TMR} = \frac{R_{AP} - R_{P}}{R_{P}} = \frac{I_P - I_{AP}}{I_P},
\]

where \(R_{AP}\) and \(R_{P}\) are the resistances across the stacked configuration when the magnetizations of the ferromagnetic layers are parallel and antiparallel to each other, \(I_P\) and \(I_{AP}\) are the total currents across the devices when the magnetization of the ferromagnetic layer is in parallel (P) and antiparallel (AP) states. The SIE can be calculated by

\[
\text{SIE} = \frac{|I_{P} - I_{AP}|}{|I_{P} + I_{AP}|}.
\]

In the equilibrium state, the TMR and SIE are estimated by using the transmission coefficient at the Fermi level.

All structural relaxation calculations were performed within the framework of density-functional theory as implemented in the Vienna \textit{ab initio} simulation package (VASP). The electron-core interaction was described by the projected augmented wave pseudopotential with the general gradient approximation parameterized by Perdew, Burke, and Ernzerhof. The electron wave function was expanded in plane waves up to a cutoff energy of 500 eV, and a \(9 \times 9 \times 1\) Monkhorst–Pack \(k\)-grid was used to sample the Brillouin zone of the supercell. The convergence criterion for the electronic energy was set to be 10$^{-4}$ eV. A vacuum region of 30 Å was used in the structural relaxation calculations of the central regions to avoid interaction between adjacent slabs. Moreover, van der Waals force was included by adopting the DFT-D2 method in all structural optimizations.

All electronic transport-related calculations are performed by using Nanodcal package based on non-equilibrium Green’s function coupled with the density functional theory. A linear combination based on atomic orbital basis sets composed of double-zeta polarized functions was adopted. For self-consistent calculation, the convergence criterion of the Hamiltonian matrix is set to be 10$^{-4}$ eV.

Results and Discussion. In order to screen the influence of electrodes on the central scattering region, a long buffer layer is required to connect the left and right electrodes to the central scattering region. By calculating the real spatial potential distribution of the system center, whether the length of the buffer layer is sufficient.
The results show that the potentials on the left and right sides are smooth at the zone close to the electrode, indicating that the buffer layer can screen the influence of electrodes. In addition, there is a very high peak in the potential energy diagram corresponding to the position of h-BN, indicating that the insulating layer h-BN forms a barrier layer between MnBi$_2$Te$_4$ [as shown in Fig. S2 in the Supplementary Material].

As shown in Fig. 1, in the monolayer MnBi$_2$Te$_4$ adjacent to h-BN, if the magnetic moments of Mn atoms are along the same direction, the system is in the parallel (P) state. If the magnetic moments of Mn atoms are along the opposite directions, the system is in the antiparallel (AP) state. Meanwhile, the natural A-type antiferromagnetic configuration is set at the side with multilayer MnBi$_2$Te$_4$.[47]

Figures 2(a)–2(h) show the calculated $I$–$V$ curves as a function of bias voltage ranging from $-0.6\, \text{V}$ to $0.6\, \text{V}$ in the parallel and the antiparallel states for all MnBi$_2$Te$_4$-based MTJs. The results indicate that for any bias, the spin current always increases in both up and down channels in the Cu/MnBi$_2$Te$_4$/h-BN/MnBi$_2$Te$_4$/Cu and Cu/MnBi$_2$Te$_4$/h-BN/MnBi$_2$Te$_4$/Cu MTJs, and that of the Cu/MnBi$_2$Te$_4$/MnBi$_2$Te$_4$/Cu MTJ obviously exceeds that of the Cu/MnBi$_2$Te$_4$/h-BN/MnBi$_2$Te$_4$/Cu MTJ. As an insulator, the potential barrier formed by h-BN is much higher than that of vacuum layer, resulting in a significant decrease of current. For both structures, with the increase of bias, the spin-polarized current can be induced. When the Cu/MnBi$_2$Te$_4$/MnBi$_2$Te$_4$/Cu MTJ is in parallel state, the current in the spin-up channel increases linearly and is always larger than that in the spin-down channel for any bias. After switching the system to the antiparallel state, under positive bias, the current in the spin-up channel increases linearly and the spin-polarized current can be induced. When the bias exceeds $0.4\, \text{V}$ or $-0.2\, \text{V}$, the spin-polarized current gradually increases. In the antiparallel state, the spin-polarized current is also suppressed when the bias is within the range from $-0.1\, \text{V}$ to $0.3\, \text{V}$. By further increasing the bias, the spin-polarized current can be observed. Therefore, these results indicate that there is a prominent switching effect in both parallel and antiparallel states.
The TMR of our MnBi$_2$Te$_4$-based MTJs is displayed in Fig. 2(i). At the equilibrium state, the TMR ratios of Cu/MnBi$_2$Te$_4$/MnBi$_2$Te$_4$/Cu and Cu/MnBi$_2$Te$_4$/h-BN/MnBi$_2$Te$_4$/Cu can reach 77.9% and 76%, respectively. In contrast, they can only reach 1.6% and 16.3% in Cu/MnBi$_2$Te$_4$/h-BN/2 MnBi$_2$Te$_4$/Cu and Cu/MnBi$_2$Te$_4$/h-BN/3 MnBi$_2$Te$_4$/Cu. With the increase of bias voltage, the TMR ratio decreases gradually and tends to be vanishing in Cu/MnBi$_2$Te$_4$/MnBi$_2$Te$_4$/Cu. For the Cu/MnBi$_2$Te$_4$/h-BN/2 MnBi$_2$Te$_4$/Cu system, when the positive bias increases to 0.6 V, the total current of antiparallel state increases prominently and exceeds the total current of parallel state, giving rise to a negative TMR ratio up to −30.6%. After the negative bias is applied, the current of parallel and antiparallel states will increase gradually in the bias range of (−0.2, −0.6 V), and the total current at the parallel state is larger than that at the antiparallel state, resulting in an enhanced TMR effect. For the Cu/MnBi$_2$Te$_4$/h-BN/3 MnBi$_2$Te$_4$/Cu MTJ, when the bias voltage increases up to 0.6 V, the current at the parallel state increases obviously, but the current at the antiparallel state decreases, resulting in a high TMR ratio about 91.1%. After the negative bias is applied, the current at the parallel state increases clearly at the bias voltage of −0.2 V, while the current at the antiparallel state is very limited. At the bias of −0.2 V, Cu/MnBi$_2$Te$_4$/h-BN/3 MnBi$_2$Te$_4$/Cu possesses the maximum TMR ratio of 162.6%. It is well known that MTJs with TMR ratios exceeding 100% can be used to produce both magnetic field sensors (key components of hard drives) and magnetoresistive random access memories. Therefore, the Cu/MnBi$_2$Te$_4$/h-BN/3 MnBi$_2$Te$_4$/Cu MTJ can be considered as a superior candidate to build spintronic devices.

Spin polarization is a key factor to determine the TMR performance, because a high spin-polarized current is essential to form a high magnetoresistance. Figure 2(j) plots the SIE of all MnBi$_2$Te$_4$-based MTJs at the parallel and antiparallel states, respectively. For the equilibrium state, the SIE of the parallel state can reach 73.5% and 66.5% for Cu/MnBi$_2$Te$_4$/MnBi$_2$Te$_4$/Cu and Cu/MnBi$_2$Te$_4$/h-BN/MnBi$_2$Te$_4$/Cu MTJs, respectively. When Cu/MnBi$_2$Te$_4$/h-BN/3 MnBi$_2$Te$_4$/Cu is at the antiparallel state, the SIE can reach 80.9% under the bias voltage of 0.4 V. When Cu/MnBi$_2$Te$_4$/h-BN/3 MnBi$_2$Te$_4$/Cu is at the parallel state, a higher SIE can reach up to 83.3% at −0.2 V.

To visualize the spin-dependent transport properties, the real-space projected density of states along the direction (z-axis) of the parallel and antiparallel states of Cu/MnBi$_2$Te$_4$/MnBi$_2$Te$_4$/Cu and Cu/MnBi$_2$Te$_4$/h-BN/MnBi$_2$Te$_4$/Cu.

Fig. 3. The spin-resolved projected density of states along the transport direction (z-axis) of the parallel and antiparallel states of Cu/MnBi$_2$Te$_4$/MnBi$_2$Te$_4$/Cu and Cu/MnBi$_2$Te$_4$/h-BN/MnBi$_2$Te$_4$/Cu.

To further understand the TMR effect and the SIE, we investigate the non-equilibrium quantum transport properties by calculating the transmission coefficient at different bias voltages of these MTJs. According to Eq. (1), the current is finally determined by the transmission coefficient entering the integration interval. Figure 3 shows the transmission coefficients of the Cu/MnBi$_2$Te$_4$/MnBi$_2$Te$_4$/Cu...
MTJ as a function of energy at different bias voltages (0.0, 0.2, and 0.4 V). At the parallel state, one can find that there is an obvious spin polarization near the Fermi level, and the spin-up transmission coefficient is larger than that of spin-down. Therefore, the spin-up electrons contribute more to the transmission spectrum, leading to a significant SIE at the equilibrium state. The corresponding SIE and TMR, together with the negative differential resistance, may pave the way for development of high-performance spin-based magnetic detection and high-frequency logic devices.

Fig. 4. Transmission coefficients as a function of energy at different bias voltages (0.0, 0.2, and 0.4 V) for Cu/MnBi₂Te₄/Cu. Insets correspond to enlarged views of transmission coefficients near the Fermi level.

In summary, the electronic transport properties of Cu/MnBi₂Te₄/Te/MnBi₂Te₄/Cu and Cu/MnBi₂Te₄/h-BN/n-MnBi₂Te₄/Cu (n = 1, 2, 3) MTJs are systematically studied by using nonequilibrium Green’s function and the density-functional theory. At both parallel and antiparallel states, Cu/MnBi₂Te₄/h-BN/n-MnBi₂Te₄/Cu (n = 2, 3) MTJs exhibit huge potential as switching devices at the bias range of (0.0, 0.3 V). Particularly, the maximum TMR ratio of Cu/MnBi₂Te₄/h-BN/3-MnBi₂Te₄/Cu can reach 162.6%. At the antiparallel state, there is a significant negative differential resistance effect in Cu/MnBi₂Te₄/h-BN/3-MnBi₂Te₄/Cu. Our results provide important theoretical guidance for further study of MnBi₂Te₄-based van der Waals magnetic tunnel junctions.

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