

Angular-dependent tunneling magnetoresistance in a tunnel junction with ferromagnetic and noncollinear antiferromagnetic electrodes

Qing-Qing Luo,^{1,2} Xiao-Yan Guo,^{1,*} Hang Zhou,^{1,3} Gautam Gurung,⁴ Jun-Min Xu⁵,⁶ Wen-Jian Lu¹, Yu-Ping Sun^{1,6,7}, Evgeny Y. Tsymbal^{8,†} and Ding-Fu Shao^{1,‡}

¹Key Laboratory of Materials Physics, *Institute of Solid-State Physics, HFIPS, Chinese Academy of Sciences, Hefei 230031, China*

²*University of Science and Technology of China, Hefei 230026, China*

³*Institute of Physical Science and Information Technology, Anhui University, Hefei 230601, China*

⁴*Trinity College, University of Oxford, Oxford OX1 3BH, United Kingdom*

⁵*Key Laboratory of Materials Physics, Ministry of Education, School of Physics, Zhengzhou University, Zhengzhou 450001, China*

⁶*Anhui Key Laboratory of Low-Energy Quantum Materials and Devices, High Magnetic Field Laboratory, HFIPS, Chinese Academy of Sciences, Hefei 230031, People's Republic of China*

⁷*Collaborative Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210093, People's Republic of China*

⁸*Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, Nebraska 68588-0299, USA*



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Magnetic tunnel junctions (MTJs) based on ferromagnetic (FM) metal electrodes exhibit a tunneling magnetoresistance (TMR) effect, which can be well understood using a model of two spin-conduction channels and spin conservation in the tunneling process. Recently, TMR has been predicted and observed in antiferromagnetic (AFM) tunnel junctions (AFMTJs) based on noncollinear AFM electrodes, promising for high-speed and high-density spintronic applications. These findings challenge the conventional mechanism of TMR due to generally no spin conservation in noncollinear AFM metals. Here, we explore spin-polarized tunneling in an $\text{Mn}_3\text{GaN}/\text{SrTiO}_3/\text{SrRuO}_3$ (001) MTJ, where the reference layer is a noncollinear AFM Mn_3GaN electrode and the free layer is a collinear FM SrRuO_3 electrode. Based on quantum-transport calculations, we predict that the rotation of FM magnetization of SrRuO_3 leads to the angular-dependent TMR being largely controlled by the matching of the average momentum-dependent spin polarization of the two electrodes. These results demonstrate that despite broken spin conservation in the tunneling process, the momentum-dependent spin polarization of the electrodes is a valuable quantity which can be used for elucidating TMR in MTJs with noncollinear AFM electrodes.

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I. INTRODUCTION

Spintronics utilizes the spin-dependent transport properties of magnetic materials for information technology [1]. Among the existing spintronic devices are magnetic tunnel junctions (MTJs) [2–5]. Due to their strong magnetoresistive response, MTJs are widely used in magnetic random-access memories and magnetic-field sensors. A typical MTJ is composed of two ferromagnetic (FM) electrodes separated by a nonmagnetic insulating barrier layer. A charge current, spin polarized by one FM electrode along its magnetization direction, tunnels across the barrier to another FM electrode, where it encounters electronic states that are spin polarized along the magnetization direction of this electrode. As a result, tunneling conductance depends on the relative magnetization orientation of the two electrodes, known as the tunneling magnetoresistance (TMR) effect [6–8]. The angular dependence

of $\text{TMR}(\alpha) = \frac{G(\alpha) - G_{\min}}{G_{\min}}$, where α is the angle between magnetizations of two FM electrodes, $G(\alpha)$ is conductance of the MTJ as a function of α , and $G_{\min}$ is the minimal conductance, stems from the spinor transformation under spin rotation leading to $\cos \alpha$ dependence of $\text{TMR}(\alpha)$ [3]. Recently, efforts have been made to implement van der Waals (vdW) materials in ultrathin MTJs [9–16].

While ferromagnets with their high degree of spin polarization are known to be valuable for spintronics, recently, antiferromagnets have emerged as promising alternative materials [17–19]. Due to their stability against magnetic perturbations, absence of stray fields, and ultrafast dynamics, antiferromagnets can potentially replace ferromagnets. To realize this potential, efficient electric control and detection of the antiferromagnetic (AFM) Néel vector are required. These functionalities can be realized using AFM tunnel junctions (AFMTJs) as core spintronic devices [20–25]. Previous experiments considered vdW AFM insulators as a tunnel barrier for a spin-filter AFMTJ, where an applied magnetic field switches the AFM state of the barrier to a metastable FM state, generating a giant spin-filter TMR effect [26–33]. Proper twisting or vdW heterostructuring may make such device nonvolatile

*Contact author: xyguo@issp.ac.cn

†Contact author: tsymbal@unl.edu

‡Contact author: dfshao@issp.ac.cn

[34,35]. However, the low Néel temperatures of vdW AFM insulators hinder the realistic applications of the vdW spin-filter AFMTJs.

AFMTJs based on AFM electrodes are more practical, since there are numerous room temperature metallic anti-ferromagnets existing in nature. Theoretically, to obtain a sizable TMR, AFMTJs need to employ AFM electrodes exhibiting momentum-dependent and/or sublattice-dependent transport spin polarization. The former includes noncollinear antiferromagnets [36–39] and collinear antiferromagnets with altermagnetic [40–50] or nonaltermagnetic [51] spin splitting. The latter can host A-, C-, or X-type AFM stacking in real space with strong intrasublattice coupling supportive to the Néel spin currents [52,53]. Experimentally, sizable TMR effects have been demonstrated in AFMTJs using noncollinear Mn_3Pt [54,55] and Mn_3Sn [56] electrodes.

The prediction [37] and observation [54–56] of the sizable TMR in AFMTJs based on noncollinear electrodes had raised an interesting fundamental question of how the large TMR can occur in noncollinear systems where spin is not conserved in the transport process. The answer to this question was recently found by Gurung *et al.* [57], who predicted that at certain transverse wave vectors $\mathbf{k}_\parallel$, noncollinear antiferromagnets can be characterized by the $\mathbf{k}_\parallel$ -dependent wave functions with uniquely defined spin states, which enforces spin conservation at these transverse wave vectors. As a result, AFMTJs with two identical noncollinear AFM electrodes may lead to the extraordinary TMR, due to the nearly perfect spin polarization of the two electrodes at these $\mathbf{k}_\parallel$.

The situation is, however, different for AFMTJs with dissimilar electrodes, where there is no match between the spin states of the conduction channels at a given $\mathbf{k}_\parallel$. In this case, the spin state of the transport electrons is not expected to be conserved and thus it is not clear whether a sizable TMR can occur in such AFMTJs. Also, the angular dependence of TMR may deviate from the standard $\cos \alpha$ dependence.

To explore this behavior, in this work, we investigate TMR in an MTJ with one electrode being a noncollinear AFM metal and another a collinear FM metal. This kind of MTJ is the simplest example where matching (mismatching) of a complex spin texture of a noncollinear antiferromagnet and a simpler spin texture of a collinear ferromagnet can be studied as a function of the rotation angle of FM magnetization. Using first-principles quantum-transport calculations on Mn_3GaN and SrRuO_3 as representative examples of the noncollinear AFM and collinear FM electrodes, respectively, and SrTiO_3 as a barrier layer, we investigate the effects of the momentum-dependent spin texture of the electrodes on the angular dependence of TMR in a $\text{Mn}_3\text{GaN}/\text{SrTiO}_3/\text{SrRuO}_3(001)$ MTJ. Although the two electrodes are different, we predict a sizable magnetoresistive response that is controlled by matching the in-plane components of their momentum-dependent transport spin polarizations. The “classical” $\cos \alpha$ dependence of TMR is reproduced, where α is the angle between the magnetization of SrRuO_3 and the effective transport spin polarization of Mn_3GaN that is determined by the spin texture of $\text{Mn}_3\text{GaN}(001)$ near the center of its Brillouin zone. This result shows that MTJs with a free FM layer and a noncollinear AFM layer as electrodes can be used for magnetic-field sensors.

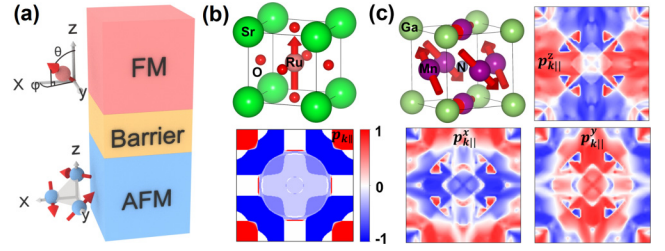


FIG. 1. (a) Schematic of an MTJ with a FM electrode and a noncollinear AFM electrode. (b) Atomic and magnetic structure of FM SrRuO_3 and its $\mathbf{k}_\parallel$ -dependent spin polarization $p_{\mathbf{k}_\parallel}$ at E_F in the 2DBZ. (c) Atomic and magnetic structure of noncollinear AFM Mn_3GaN and its $\mathbf{k}_\parallel$ -dependent spin polarization $p_{\mathbf{k}_\parallel}$ at E_F in the 2DBZ.

II. THEORETICAL METHODS

The calculations of the electronic properties (electronic bands, density of states, and Fermi surfaces) of the $\text{Mn}_3\text{GaN}/\text{SrTiO}_3/\text{SrRuO}_3(001)$ heterostructure are performed using density functional theory (DFT) as implemented in the Vienna *Ab initio* simulation package (VASP) [58,59]. The exchange-correlation potential is described through the Perdew-Burke-Ernzerhof formula within the generalized gradient approximation [60]. The kinetic energy cutoff is set to 550 eV and the k -point grid of $10 \times 10 \times 1$ is adopted for integration over the first Brillouin zone (BZ).

The transport properties ($\mathbf{k}_\parallel$ -dependent and total transmissions) of $\text{Mn}_3\text{GaN}/\text{SrTiO}_3/\text{SrRuO}_3$ MTJs are calculated using the nonequilibrium Green's function formalism (DFT+NEGF method) [61,62], as implemented in QUANTUMATK, Synopsys QUANTUMATK [63]. The atomic structures are relaxed by VASP using the nonrelativistic Fritz-Haber-Institute pseudopotentials within a single-zeta-polarized basis. To eliminate a mismatch of the Fermi level between the electrodes and the central region, the cut-off energy is set to be 75 Ry and the k -point mesh is set to be $11 \times 11 \times 101$ to perform the self-consistent calculations. The transmission is calculated using a k -point mesh of 201×201 in the two-dimensional BZ (2DBZ) of the $\text{Mn}_3\text{GaN}/\text{SrTiO}_3/\text{SrRuO}_3(001)$ MTJ. The spin-orbit coupling is not included in the calculations.

III. RESULTS

Figure 1(a) schematically shows an MTJ with collinear FM and noncollinear AFM electrodes. The FM electrode is represented by SrRuO_3 [Fig. 1(b)], a perovskite metal with the FM ground state [64–66]. For the collinear magnet, we define the $\mathbf{k}_\parallel$ -resolved transport spin polarization $p_{\mathbf{k}_\parallel}$ as follows:

$$p_{\mathbf{k}_\parallel} = \frac{N_{\mathbf{k}_\parallel}^\uparrow - N_{\mathbf{k}_\parallel}^\downarrow}{N_{\mathbf{k}_\parallel}^\uparrow + N_{\mathbf{k}_\parallel}^\downarrow}, \quad (1)$$

where $\mathbf{k}_\parallel = (k_x, k_y)$ is the transverse wave vector in the 2DBZ of $\text{SrRuO}_3(001)$ [Fig. 1(b)], and $N_{\mathbf{k}_\parallel}^\uparrow$ and $N_{\mathbf{k}_\parallel}^\downarrow$ are the number of conduction channels of up- ($\uparrow$) and down- ($\downarrow$) spin electrons, respectively, calculated at the Fermi energy (E_F) and $\mathbf{k}_\parallel$. As seen from Fig. 1(b), the maximal $|p_{\mathbf{k}_\parallel}| = 100\%$ is found around the corners of the 2DBZ, whereas $p_{\mathbf{k}_\parallel}$ is

smaller ($\approx -33\%$) around the zone center and vanishes in the area around the $k_x = 0$ and $k_y = 0$ lines away from the zone center. The $\mathbf{k}_{\parallel}$ -resolved spin polarization can be considered as a vector $\mathbf{p}_{k_{\parallel}}$, which is aligned (or antialigned) along the direction of the magnetic moment of SrRuO₃.

The noncollinear AFM electrode is represented by antiperovskite Mn₃GaN [Fig. 1(c)], which has a Γ_{5g} noncollinear AFM configuration, where Mn magnetic moments form a 120° chiral alignment within the (111) kagome plane [67]. Such a noncollinear magnetic ordering breaks $\hat{P}\hat{T}$ and D_n spin-space symmetries, where $\hat{P}$ is space inversion, $\hat{T}$ is time reversal, and D_n represents rotations and reflections within a dihedral group with n being any positive integer [68], resulting in a spin-polarized Fermi surface [see Supplemental Material Fig. S1(b) [69]] and hence spin-polarized conduction channels.

Contrary to collinear magnets, for noncollinear antiferromagnets, Eq. (1) cannot be used as the definition of the $\mathbf{k}_{\parallel}$ -resolved transport spin polarization. A more appropriate definition of an effective spin polarization for noncollinear systems is given in [57] as follows:

$$\mathbf{p}_{k_{\parallel}} = \frac{\sum_n s_{nk_{\parallel}}}{\sum_n |s_{nk_{\parallel}}|}, \quad (2)$$

where

$$s_{nk_{\parallel}} = \frac{l_z}{2\pi} \int \langle \psi_{nk} | s | \psi_{nk} \rangle \delta(E_{nk} - E_F) dk_z. \quad (3)$$

Here l_z is the lattice constant of the electrode along the transport direction and $\langle \psi_{nk} | s | \psi_{nk} \rangle$ is the spin expectation value for band n of energy E_{nk} at wave vector $\mathbf{k} = (\mathbf{k}_{\parallel}, k_z)$. For collinear magnets, this definition of $\mathbf{p}_{k_{\parallel}}$ is equivalent to that given by Eq. (1). However, in contrast to collinear magnets, in noncollinear magnets, $\mathbf{p}_{k_{\parallel}}$ is a vector with variable directions and magnitudes. Figure 1(c) shows the calculated i components ($i = x, y, z$) of $\mathbf{p}_{k_{\parallel}}$ ($p_{k_{\parallel}}^i$), which are consistent with those obtained previously using a different code [57]. As has been discussed in [57], $p_{k_{\parallel}}^z$ is antisymmetric with respect to the diagonals parallel to k_{110} and $k_{\bar{1}10}$ in the 2DBZ and also obeys the relationship $p_{k_x, k_y}^x = -p_{k_y, k_x}^y$. We find that the magnitude of $p_{k_{\parallel}}^x$ ($p_{k_{\parallel}}^y$) is relatively large around $k_y = 0$ ($k_x = 0$). A nearly perfect $\mathbf{p}_{k_{\parallel}}$ with $|\mathbf{p}_{k_{\parallel}}| = 100\%$ appears in a broad area of the 2DBZ, especially around the $k_x = 0$ and $k_y = 0$ lines away from the zone center (Fig. S1) [69].

As has been discussed in [57], a perfect spin polarization in a noncollinear AFM crystal for a given $\mathbf{k}_{\parallel}$ implies that, at this $\mathbf{k}_{\parallel}$, there are no bands with different spin orientation for the current-carrying electrons to be scattered to, which is effectively equivalent to the spin-conservation condition. As a result, in an AFMTJ with two identical noncollinear AFM electrodes, such as Mn₃GaN, matching of the nearly perfect $\mathbf{p}_{k_{\parallel}}$ in the two electrodes results in an extraordinary TMR. In our case of different electrodes, however, the area of $|\mathbf{p}_{k_{\parallel}}| = 100\%$ in Mn₃GaN is largely overlapped with the area of small or vanishing $p_{k_{\parallel}}$ in SrRuO₃. It is not, therefore, obvious, in this case, if the spin state of the transport electrons is expected to be conserved and how the TMR ratio will depend on the magnetization orientation of SrRuO₃.

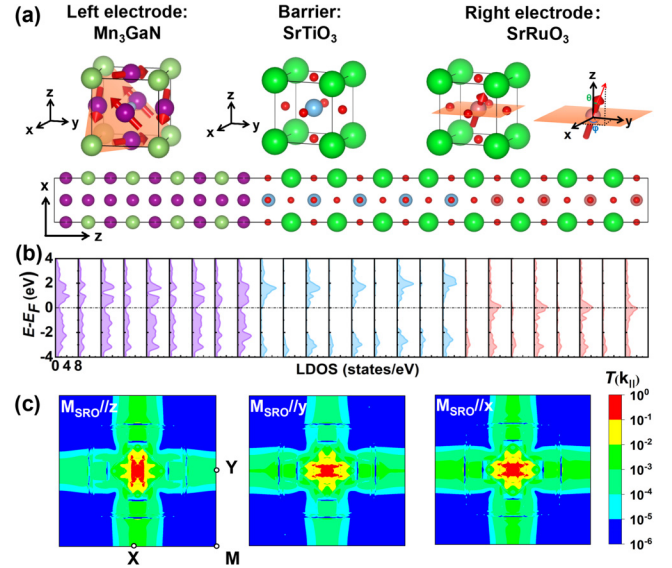


FIG. 2. (a), (b) Atomic structure of the electrodes, barrier, and the heterostructure used in the quantum-transport calculation (a) and the layer-resolved density of states (LDOS) (b) of the Mn₃GaN/SrTiO₃/SrRuO₃(001) heterostructure. (c) The calculated $\mathbf{k}_{\parallel}$ -resolved transmission of the Mn₃GaN/SrTiO₃/SrRuO₃ MTJ for magnetization of SrRuO₃ $\mathbf{M}_{\text{SRO}}$ along the z , y , and x directions.

To answer these questions, we assemble an Mn₃GaN/SrTiO₃/SrRuO₃(001) MTJ and perform first-principles calculations for its electronic structure as described in Sec. II. Our calculations reveal that the lattice parameters of SrRuO₃ and Mn₃GaN are 3.985 and 3.84 Å, respectively, both being consistent with the previous theoretical results [70–72]. In experiments, epitaxial Mn₃GaN and SrRuO₃ films can be grown on perovskite substrates, such as SrTiO₃, with atomically sharp interfaces [73,74]. Consequently, high-quality crystalline Mn₃GaN/SrTiO₃/SrRuO₃(001) MTJs are feasible in practice.

Figure 2(a) shows an Mn₃GaN/SrTiO₃/SrRuO₃(001) heterostructure, which is used for constructing MTJs. It consists of a 4.5-unit-cell SrTiO₃(001) barrier layer positioned between a 4.5-unit-cell Mn₃GaN(001) layer and a 4-unit-cell SrRuO₃(001) layer. To simulate epitaxial growth, the in-plane lattice constant of the MTJ is fixed to be the calculated lattice constant of SrTiO₃, i.e., $a = 3.94$ Å. Under this constraint, the atomic positions of the heterostructure are relaxed. The presence of strain does not qualitatively influence the $\mathbf{k}_{\parallel}$ -resolved spin polarization of Mn₃GaN and SrRuO₃, as shown in Fig. S3 [69]. Figure 2(b) shows the layer-resolved density of states (DOS) of the Mn₃GaN/SrTiO₃/SrRuO₃(001) heterostructure. Notably, the Fermi energy (E_F) of the system lies near the conduction band minimum of SrTiO₃, while it is anticipated to be well within the band gap of the insulator. This result originates from the well-known deficiency of DFT in describing excited states, leading to the underestimated band gap of SrTiO₃. We find, however, that this deficiency does not influence our conclusions, as the results presented below do not show qualitative changes if the band gap of SrTiO₃ is corrected by a large Hubbard U (Figs. S5 and S6) [69,75,76].

The control of the AFM Néel vector is crucial for information write-in AFM-based devices, which remains a challenge in the AFM spintronics [17–19]. In an MTJ with AFM and FM electrodes, the write-in operation can be performed by rotating FM magnetization using a magnetic field or a spin torque [24,25]. Therefore, in the calculations of the $\text{Mn}_3\text{GaN}/\text{SrTiO}_3/\text{SrRuO}_3$ MTJ, we fix the magnetic structure Mn_3GaN and rotate the magnetization of SrRuO_3 , $\mathbf{M}_{\text{SRO}}$, as schematically shown in Fig. 1(a). Figure 2(c) shows the $k_{\parallel}$ -resolved transmission, $T_{k_{\parallel}}$, calculated in the 2DBZ at E_F , when $\mathbf{M}_{\text{SRO}}$ is oriented along the x , y , and z directions. We observe that $T_{k_{\parallel}}$ forms a cross pattern, reflecting the distribution of the lowest decay rate of $\text{SrTiO}_3(001)$ in the 2DBZ [57,77]. The largest transmission $T_{k_{\parallel}}$ is concentrated near the zone center. It forms an H-shaped hot spot, which changes its orientation depending on whether $\mathbf{M}_{\text{SRO}}$ is out of plane ($\mathbf{M}_{\text{SRO}} \parallel z$) or in plane ($\mathbf{M}_{\text{SRO}} \parallel x, y$).

The H-shaped pattern of the hot spot can be understood by matching the $k_{\parallel}$ -dependent transport spin polarization of the two electrodes. For $\mathbf{M}_{\text{SRO}}$ along the z direction, $p_{k_{\parallel}}^z = p_{k_{\parallel}}$ is negative for SrRuO_3 around the zone center [Fig. 1(b)], while the $p_{k_{\parallel}}^z$ component is positive (negative) for Mn_3GaN around $k_y = 0$ ($k_x = 0$) [Fig. 1(c)]. Therefore, there is a mismatch of $p_{k_{\parallel}}^z$ for SrRuO_3 and Mn_3GaN around $k_y = 0$, suppressing transmission in this region and leading to the H-shaped pattern of $T_{k_{\parallel}}$. For $\mathbf{M}_{\text{SRO}}$ along the x direction, the H-shaped pattern is rotated by 90° . This is because $p_{k_{\parallel}}^x = p_{k_{\parallel}}$ of SrRuO_3 and $p_{k_{\parallel}}^x$ of Mn_3GaN are both negative, matching around $k_y = 0$, while $p_{k_{\parallel}}^y = 0$ for SrRuO_3 is mismatched to positive $p_{k_{\parallel}}^y$ for Mn_3GaN suppressing $T_{k_{\parallel}}$ around $k_x = 0$ away from the zone center. These results indicate that although $\mathbf{p}_{k_{\parallel}}$ of SrRuO_3 is reduced near the zone center and it can only match a component of $\mathbf{p}_{k_{\parallel}}$ of Mn_3GaN , it is sufficient to generate non-negligible differences in the transmission.

We therefore expect that rotation of the magnetization of SrRuO_3 can produce a magnetoresistive response in such MTJ. To demonstrate this and find the angular dependence of TMR, we calculate transmission of the MTJ with $\mathbf{M}_{\text{SRO}}$ pointing along different directions determined by the polar angles θ and φ , where the former denotes the angle between $\mathbf{M}_{\text{SRO}}$ and the positive z axis, and the latter denotes the angle between the projection of $\mathbf{M}_{\text{SRO}}$ on the $x-y$ plane and the positive x axis [Fig. 1(a)]. A TMR ratio as a function of angles θ and φ is defined by

$$\text{TMR}(\theta, \varphi) = \frac{T(\theta, \varphi) - T_{\min}}{T_{\min}}, \quad (4)$$

where $T_{\min}$ is the minimal value of $T(\theta, \varphi)$.

Figure 3 shows the calculated transmission when $\mathbf{M}_{\text{SRO}}$ is rotated within the x - y plane, i.e., $\theta = 90^\circ$ and φ varies from -180° to 180° . In this case, the $k_{\parallel}$ -dependent polarization of SrRuO_3 is given by $\mathbf{p}_{k_{\parallel}} = (p_{k_{\parallel}} \cos \varphi, p_{k_{\parallel}} \sin \varphi, 0)$. As seen from Fig. 3(a), when φ is -45° or 135° , $T_{k_{\parallel}}$ distributions exhibit a perfect fourfold rotational symmetry, with $T_{k_{\parallel}}$ for $\varphi = -45^\circ$ being larger than that for $\varphi = 135^\circ$. This can be understood by matching $\mathbf{p}_{k_{\parallel}}$ of SrRuO_3 and Mn_3GaN . As shown in Fig. S4, for $\varphi = -45^\circ$, $\mathbf{p}_{k_{\parallel}} = (\frac{1}{\sqrt{2}}p_{k_{\parallel}}, -\frac{1}{\sqrt{2}}p_{k_{\parallel}}, 0)$ of SrRuO_3 produces a good match to $p_{k_{\parallel}}^x$ ($p_{k_{\parallel}}^y$) of Mn_3GaN

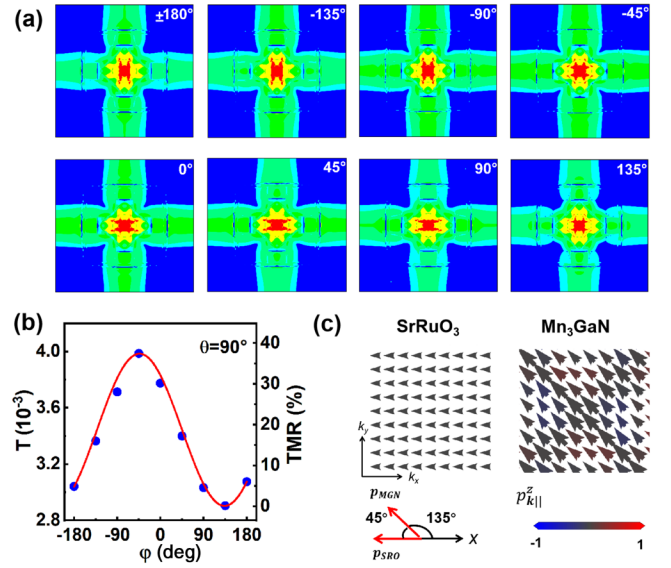


FIG. 3. (a) $k_{\parallel}$ -resolved transmission of the $\text{Mn}_3\text{GaN}/\text{SrTiO}_3/\text{SrRuO}_3(001)$ MTJ for magnetization of SrRuO_3 , $\mathbf{M}_{\text{SRO}}$, along different in-plane directions determined by the variable angle φ and fixed angle $\theta = 90^\circ$. (b) The transmission T and TMR ratio, $\text{TMR}(\varphi) = \frac{T(\varphi) - T_{\min}}{T_{\min}}$, as a function of angle φ for $\theta = 90^\circ$ calculated from DFT (dots) and fitted by a linear function of $\cos(\varphi + 45^\circ)$ (solid line). (c) Spin polarization near the center of the 2DBZ for SrRuO_3 (left) and Mn_3GaN (right).

around $k_y = 0$ ($k_x = 0$), resulting in large transmission. On the contrary, for $\varphi = 135^\circ$, $\mathbf{p}_{k_{\parallel}} = (-\frac{1}{\sqrt{2}}p_{k_{\parallel}}, \frac{1}{\sqrt{2}}p_{k_{\parallel}}, 0)$ of SrRuO_3 and $p_{k_{\parallel}}^x$ ($p_{k_{\parallel}}^y$) of Mn_3GaN are mismatched in these regions, leading to reduced $T_{k_{\parallel}}$.

As seen from Fig. 3(a), when $\mathbf{M}_{\text{SRO}}$ is rotated continuously within the x - y plane, the transmission pattern gradually changes. Overall, $T_{k_{\parallel}}$ distribution in the 2DBZ forms an H-shaped hot spot for angles $-45^\circ < \varphi < 135^\circ$ and a 90° -rotated H-shaped hot spot for angles $\varphi > 135^\circ$ and $\varphi < -45^\circ$. The transformation of these patterns can be understood based on the matching of $\mathbf{p}_{k_{\parallel}}$ of SrRuO_3 and Mn_3GaN , using arguments similar to those presented above.

Figure 3(b) shows the resulting transmission T and TMR for $\theta = 90^\circ$ as a function of angle φ . It is seen that both exhibit an oscillatory behavior which can be well fitted by a linear function of $\cos(\varphi + 45^\circ)$. Somewhat similar behavior of T and TMR as a function of angle φ is also found for $\mathbf{M}_{\text{SRO}}$ rotated away from the x - y plane ($\theta \neq 90^\circ$). This is seen from Fig. 4(a), where the φ -dependent transmission T and TMR are plotted for $\theta = 45^\circ$ and $\theta = 135^\circ$. In both cases, the calculated curves can be fitted by a linear function of $\cos(\varphi + 45^\circ)$.

Figure 4(b) visualizes the variation of TMR as a function of angles θ and φ . We find that the maximum TMR of about 40% appears for $(\theta, \varphi) = (90^\circ, -45^\circ)$. This is consistent with the symmetry transformations preserved by the Γ_{5g} configuration. First, Γ_{5g} enforces the antisymmetric distribution of $p_{k_{\parallel}}^z$ in the 2DBZ for Mn_3GaN . Therefore, $p_{k_{\parallel}}^z$ of Mn_3GaN in a half of the 2DBZ always matches that of SrRuO_3 , since $p_{k_{\parallel}}^z$ of SrRuO_3 is always symmetrically distributed. Therefore, the matching of $p_{k_{\parallel}}^z$ alone does not contribute to the transmission

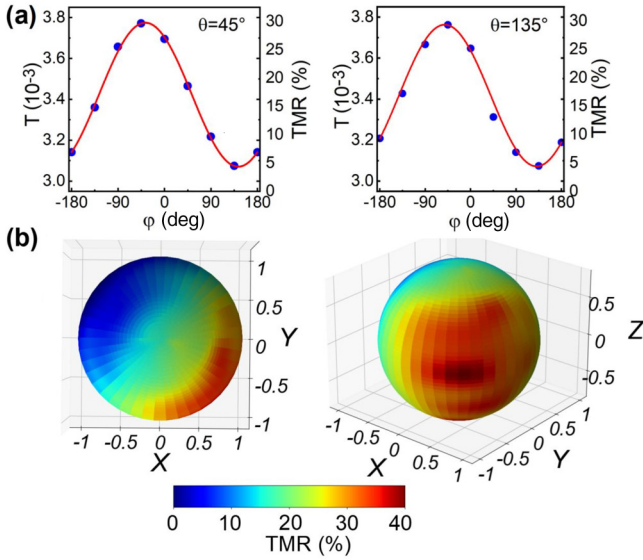


FIG. 4. (a) The φ -dependent transmission T and the associated TMR ratio $\text{TMR}(\theta, \varphi) = \frac{T(\theta, \varphi) - T_{\min}}{T_{\min}}$ for $\theta = 45^\circ$ (left) and $\theta = 135^\circ$ (right). Dots are DFT calculated values; solid lines are the fit using a linear function of $\cos(\varphi + 45^\circ)$. (b) Visualization of the angular dependence of TMR as a function of the $\mathbf{M}_{\text{SRO}}$ direction.

change for a given θ . Second, due to the symmetry-enforced relationship $p_{k_x, k_y}^x = -p_{k_y, k_x}^y$, the strongest match (mismatch) of $p_{k_{\parallel}}^{x,y}$ in Mn_3GaN and SrRuO_3 can occur only at $\varphi = -45^\circ$ (135°) for a given θ . When $\mathbf{M}_{\text{SRO}}$ lies within the $x-y$ plane ($\theta = 90^\circ$), the vanishing $p_{k_{\parallel}}^z$ ensures relatively large $p_{k_{\parallel}}^{x,y}$ of SrRuO_3 to match that of Mn_3GaN . As a result, the switching between the maximum and minimum T is associated with the 180° reversal of $\mathbf{M}_{\text{SRO}}$ along the $[\bar{1}10]$ direction.

IV. DISCUSSION

The observed angular dependence of transmission T and TMR can be understood by comparing the $\mathbf{k}_{\parallel}$ -resolved transmission patterns shown in Fig. 3(a) and the $\mathbf{k}_{\parallel}$ -resolved spin polarization $\mathbf{p}_{k_{\parallel}}$ of SrRuO_3 and Mn_3GaN shown in Figs. 1(b) and 1(c), respectively. It is seen from Fig. 3(a) that $T_{k_{\parallel}}$ is dominated by a hot spot located close to the 2DBZ center. In this region, for magnetization $\mathbf{M}_{\text{SRO}}$ pointing along the $+x$ direction, the average spin polarization $\mathbf{p}_{\text{SRO}}$ is oriented along the direction determined by the angles $(\theta_{\text{SRO}}, \varphi_{\text{SRO}}) = (90^\circ, -180^\circ)$ since $\mathbf{p}_{k_{\parallel}}$ of SrRuO_3 in this region is uniform, as depicted in Fig. 3(c) and Fig. S2. When the magnetization is rotated to have an arbitrary direction determined by the spherical angles (θ, φ) , the spin polarization is transformed: $\mathbf{p}_{\text{SRO}} = p_{\text{SRO}}(\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$. At the same time, we find that in the region of the 2DBZ close to the zone center, the in-plane components of $\mathbf{p}_{k_{\parallel}}$ of Mn_3GaN exhibit a nearly persistent spin texture, resulting in the average spin polarization $\mathbf{p}_{\text{MGN}}$ pointing along the $(\theta_{\text{MGN}}, \varphi_{\text{MGN}}) = (90^\circ, 135^\circ)$ direction, as depicted in Fig. 3(c). The angular dependence of TMR can then be understood from the matching of the average spin polarization, $\mathbf{p}_{\text{SRO}}$ and $\mathbf{p}_{\text{MGN}}$, of the electrodes. This situation is reminiscent of that for an MTJ with two FM electrodes. In the latter case, the angular dependence of

TMR is determined by $\text{TMR}(\alpha) = \text{TMR}_0(1 + \cos \alpha)$, where α is the angle between magnetizations (polarizations) of the two ferromagnetic electrodes [3]. Extending this result to our case, we have $\cos \alpha = \sin \theta \cos(\varphi + 45^\circ)$ and hence $\text{TMR}(\theta, \varphi) = \text{TMR}_0[1 + \sin \theta \cos(\varphi + 45^\circ)]$. This expression with $\text{TMR}_0 \approx 40\%$ describes well all the angular dependence of TMR which is calculated from first principles.

Previous calculations suggested that matching of the nearly perfect $\mathbf{p}_{k_{\parallel}}$ in AFMTJs with identical noncollinear AFM electrodes can result in the extraordinary TMR [57]. This is due to the spin being conserved for conduction channels with perfect $\mathbf{p}_{k_{\parallel}}$, making TMR very large for an AFMTJ where such channels dominate transmission. In the current case, the highest tunneling transmission occurs in the region of the 2DBZ where Mn_3GaN does not have perfect $\mathbf{p}_{k_{\parallel}}$. This implies the presence of several conduction channels with different spin orientations at a given wave vector $\mathbf{k}_{\parallel}$. In this case, the incoming electron with a given spin state can be transmitted to different conduction channels of Mn_3GaN , implying that the spin is not conserved in the tunneling process. Nevertheless, despite this complexity, our calculations suggest that the TMR can be supported by matching the associated components of $\mathbf{p}_{k_{\parallel}}$, and its angular dependency can be reasonably well understood based on the model where the relative angle between the average spin polarization in the electrodes determines the angular dependence of TMR. This result indicates that for an arbitrary tunnel junction with different magnetic electrodes the average spin polarizations of the electrodes in the $\mathbf{k}_{\parallel}$ area of high transmission can serve as qualitative measure for predicting TMR and its angular dependence.

The calculated TMR is sizable, indicating the potential of using noncollinear AFM electrodes in MTJs where the two electrodes are nonidentical. It is worth noting that real devices inevitably contain disorder and spin-orbit coupling which usually suppress TMR. However, it is reasonable to expect a much larger TMR for FM electrodes with spin polarization being greater than that of SrRuO_3 , where the disorder and spin-orbit coupling may not generate a significant influence on TMR. Indeed, a sizable $\text{TMR} > 100\%$ has been experimentally observed in an $\text{Mn}_3\text{Sn}/\text{MgO}/\text{CoFeB}$ MTJ, implying the TMR in the noncollinear MTJs with dissimilar electrodes can be robust against disorder and spin-orbit coupling [78].

From a technological point of view, MTJs with a noncollinear AFM electrode and a FM electrode are less appealing for memory applications compared to all-AFM tunnel junctions, due to the unavoidable stray fields and relatively slow dynamics of ferromagnets. However, these MTJs may be suitable for sensor applications [79]. A magnetic sensor is expected to be sensitive to a weak magnetic field but does not require high density and speed. In this regard, MTJs with one FM and another AFM electrode are advantageous. An AFM electrode eliminates the need for a pinning layer and hence simplifies the MTJ structure, while a FM electrode with low anisotropy allows the response to a weak magnetic field. The angular-dependent TMR can then be used to accurately reflect the FM magnetization direction. This functionality is less recognized in the realm of AFM spintronics, but worth being addressed in the future.

V. CONCLUSIONS

Overall, an MTJ with a FM metal electrode and a noncollinear AFM electrode can give rise to a sizable magnetoresistive response, despite very different electronic and magnetic structures of the two metals. Using noncollinear AFM Mn_3GaN and FM SrRuO_3 as two representative magnetic metals, we have shown that tunneling transmission across an $\text{Mn}_3\text{GaN}/\text{SrTiO}_3/\text{SrRuO}_3(001)$ MTJ is controlled by matching the momentum-dependent spin polarization of the two electrodes. Despite the broken spin conservation in the tunneling process, we have demonstrated that the angular dependence of TMR in response to the magnetization rotation of SrRuO_3 largely followed the “classical” $\cos\alpha$ behavior, where α is the angle between magnetization of SrRuO_3 and the average spin polarization of Mn_3GaN in the 2DBZ region of high transmission. These results suggest the momentum-dependent spin polarization of the electrodes is a valuable quantity which can be used for an understanding of TMR in AFMTJs with noncollinear AFM electrodes. Our results also show that MTJs with a free FM layer and a noncollinear AFM layer as electrodes can be used for magnetic-field sensors.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

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