



Current Perspectives

Magnetic reconstruction induced magnetoelectric coupling and spin-dependent tunneling in Ni/KNbO₃/Ni multiferroic tunnel junctions

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ABSTRACT

We investigate the magnetoelectric coupling and spin-polarized tunneling in Ni/KNbO₃/Ni multiferroic tunnel junctions with asymmetric interfaces based on density functional theory. The junctions have two stable polarization states. We predict a peculiar magnetoelectric effect in such junctions originating from the magnetic reconstruction of Ni near the KO-terminated interface. This reconstruction is induced by the reversal of the ferroelectric polarization of KNbO₃. Furthermore, the change in the magnetic ordering filters the spin-dependent current. This effect leads to a change in conductance by about two orders of magnitude. As a result we obtain a giant tunneling electroresistance effect. In addition, there exist sizable tunneling magnetoresistance effects for two polarization states.

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1. Introduction

A multiferroic tunnel junction (MFTJ) can be constructed with ferromagnetic electrodes separated by a ferroelectric barrier [1]. There are rich interesting physical phenomena in MFTJs. An interfacial magnetoelectric (ME) coupling was predicted in Fe/BaTiO₃ junctions [2]. The strong hybridization between the Ti 3d band and the minority spin Fe 3d band induced large magnetic moments on interfacial Ti atoms, which is altered by the polarization orientation. Researchers have confirmed this prediction experimentally by means of element selective X-ray resonant magnetic scattering spectra [3,4]. In addition, the magnetic anisotropy at the interface of Fe/BaTiO₃ systems has also been found [5–7]. The ME effects originating from interface bonding in Fe₃O₄/BaTiO₃, Co/BaTiO₃, Co₂MnSi/BaTiO₃, and Fe/PbTiO₃ were also investigated [8–11]. Furthermore there exists another type of ME effect induced by magnetic reconstruction at the interface of MFTJs. For example, a magnetic order transition from ferromagnetic to antiferromagnetic was found at the interface of La_{0.7}Sr_{0.3}MnO₃/BaTiO₃/La_{0.6}Sr_{0.4}MnO₃ when polarization reverses [12,13]. The physical mechanism of this effect was the formation of screening charges to screen the bound charges produced by the polarization in BaTiO₃ layers. The magnetic phase transition in

ultrathin Fe films deposited on the (001) surface of 0BaTiO₃ and PbTiO₃ with TiO₂ terminations has been predicted [14]. For one monolayer Fe, the magnetic moments on Fe were enhanced compared to that of bulk Fe. The ferrimagnetic order appeared when a second Fe layer was deposited. The ferromagnetic order can be restored through adding a third Fe layer. The sign of the magnetic moments did not change with polarization reversal. The magnetovolume instability of Fe was thought to be the mechanism of this magnetic phase transition. In Fe/Au/Fe/PbTiO₃, the reversal of polarization led to a 180° switching of the magnetization of the Fe layer originated from the interlayer exchange coupling [15].

On the other hand, the physical phenomenon of transport in MFTJs is very attractive. The electron tunneling in MFTJs depends on the magnetization configuration of electrodes. Thus a MFTJ exhibits tunneling magnetoresistance (TMR). In addition, the orientation of ferroelectric polarization can also control the tunneling current. This effect is known as tunneling electroresistance (TER). Hence the TER and TMR can coexistence in MFTJs [1]. There are a number of theoretical and experimental studies on the spin-dependent transport in MFTJs. Four resistance states in SrRuO₃/BaTiO₃/SrRuO₃ MFTJs have been predicted. The MFTJs with asymmetric interfaces were found to have two polarization states [16]. The Δ₁ and Δ₅ states in the band gap of BaTiO₃ and their variations with polarization reversal dominated the conductance. Garcia et al. succeeded in controlling the carrier spin polarization through polarization reversal in Fe/BaTiO₃/La_{0.67}Sr_{0.33}MnO₃ junctions [17]. Both the TER and TMR have been observed in La_{0.7}

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$\text{Sr}_{0.3}\text{MnO}_3/(\text{Ba}, \text{Sr})\text{TiO}_3/\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ MFTJs experimentally at room temperature [18]. Another interesting phenomenon appeared in, mentioned earlier, $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{BaTiO}_3/\text{La}_{0.6}\text{Sr}_{0.4}\text{MnO}_3$ MFTJs [13]. A ferroelectrically induced change of magnetic order produced a giant TER effect. Yin et al. observed a similar effect in $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{BaTiO}_3/\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3/\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ junctions experimentally [19].

In this paper, we investigate the electronic structure and spin-dependent electron tunneling in Ni/KNbO₃/Ni MFTJs with asymmetric interfaces. The junctions have two stable polarization states. We find a magnetic reconstruction in such MFTJs with the switching of ferroelectric polarization. This leads to a strong ME coupling. This phenomenon has an important influence on the spin-dependent transport. As a result, giant TER effects are obtained. Furthermore, there are sizable TMR effects for two polarization states.

2. Methods

The Ni/KNbO₃/Ni MFTJs consist of Ni layers separated by the KNbO₃ layers containing six unit cells. We align the body-centered-cubic (bcc) Ni [110] with the [001] axis of KNbO₃. The calculated magnetic moments of bulk bcc Ni is $0.53 \mu_B$. The experimental value with the lattice constant of $2.82 \text{ \AA}$ is $0.52 \mu_B$ [20]. The in-plane lattice constant of the junction is set to be our theoretical value ($3.996 \text{ \AA}$) of bulk KNbO₃ with the tetragonal phase, which agrees with the experimental results ($3.997 \text{ \AA}$). To produce the TER effect, the KNbO₃ barriers should have two stable polarization states with opposite directions and thus MFTJs should have asymmetric interfaces. We assume that the KNbO₃ barrier has the NbO₂ termination (the O atoms on top of Ni) at the left interface and the KO termination (Ni on top of the O and K atoms) at the right interface. As shown in Fig. 1(a), for the KO termination, there are two different interfacial Ni atoms denoted as Ni1 and Ni2. The

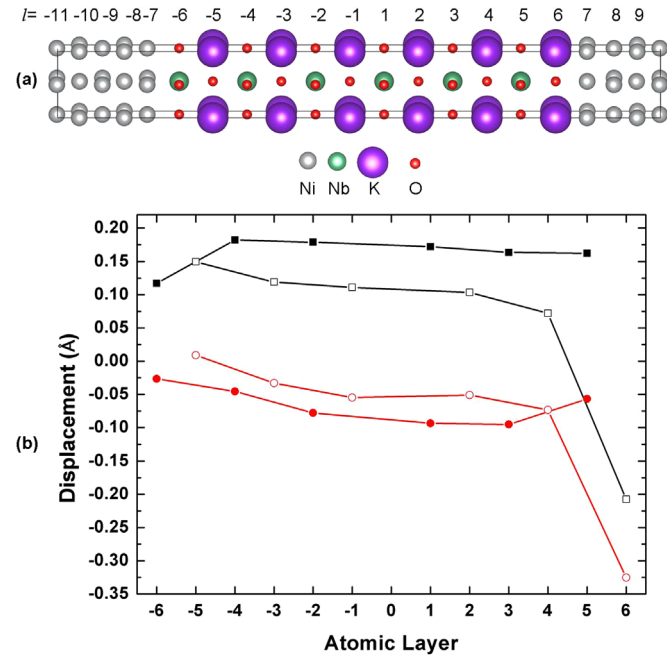


Fig. 1. (a) Atomic structure of the Ni/KNbO₃/Ni MFTJ. The atomic layer numbers (l) are also shown. (b) The relative displacements of Nb and K with respect to O. Filled (open) red circle symbols denote Nb–O (K–O) displacements with the polarization pointing to the left. Filled (open) black square symbols denote the Nb–O (K–O) displacements with the polarization pointing to the right. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Ni1 and Ni2 are on top of O and K respectively. The polarization of the KNbO₃ barrier may point to the right (P_+) or the left (P_-). Fig. 1(a) illustrates the atomic structure of the Ni/KNbO₃/Ni MFTJ.

We use the Vienna *ab initio* simulation package (VASP) [21–23] to calculate the atomic and electronic structures of Ni/KNbO₃/Ni MFTJs. The Perdew–Burke–Ernzerhof (PBE) [24] generalized gradient approximation (GGA) is employed with the energy cutoff 500 eV. We relax the structure until the Hellmann–Feynman forces are less than $20 \text{ meV/\AA}$ with a Monkhorst–Pack grid [25] of $6 \times 6 \times 1$. A $12 \times 12 \times 2$ grid is used for the density of states (DOS) calculations.

We use the Quantum ESPRESSO package [26] to calculate the spin-dependent tunneling conductance of the Ni/KNbO₃/Ni MFTJs. The atomic structure shown in Fig. 1(a) is used as the scattering region. Two semi-infinite Ni electrodes are attached on two sides of the junction when we calculate the conductance. The ballistic conductance for junctions is given by the Landauer–Büttiker formula [27]:

$$G = \frac{e^2}{h} \sum_{\sigma, K_{\parallel}} T_{\sigma}(K_{\parallel}) \quad (1)$$

where $T_{\sigma}(K_{\parallel})$ gives the transmission probability for the electron with Bloch wave vector $K_{\parallel} = (k_x, k_y)$ corresponding to the periodicity in the plane of the junction and spin σ at the Fermi energy. The TMR ratio can be defined as

$$\text{TMR} = \frac{G_P - G_{AP}}{G_{AP}} \quad (2)$$

where $G_{AP} = G_{\uparrow\downarrow} + G_{\downarrow\uparrow}$ and $G_P = G_{\uparrow\uparrow} + G_{\downarrow\downarrow}$ are the conductance of the antiparallel and parallel magnetic configuration respectively. We denote the conductance of the majority (minority) spin channel by $G_{\uparrow\uparrow}$ ($G_{\downarrow\downarrow}$). $G_{\uparrow\downarrow}$ and $G_{\downarrow\uparrow}$ are the conductance of the minority-to-majority and majority-to-minority spin channels respectively. We define the TER ratio as

$$\text{TER} = \frac{G_+ - G_-}{\min(G_+, G_-)} \quad (3)$$

where G_+ and G_- are the conductance with the polarization pointing to the right and left respectively.

3. Results and discussion

3.1. Magnetic reconstruction induced ME effect

Firstly we investigate the equilibrium atomic structure of Ni/KNbO₃/Ni MFTJs. As mentioned above, the MFTJ has asymmetric interfaces. We obtain two polarization states of KNbO₃ for the MFTJ after fully relaxation. The total energy of the P_+ state is 300 meV (50 meV per unit cells of KNbO₃) lower than that of the P_- state. Fig. 1(b) gives the relative displacements in the KNbO₃ barriers. The relative K–O and Nb–O displacements in the bulk tetragonal phase KNbO₃ are 0.08 and 0.15 Å respectively. For the P_+ state, the Nb–O displacement at the left interface is 0.12 Å. While the displacement for other layers are all larger than 0.16 Å. The amplitudes of the K–O displacements are all larger than 0.10 Å except the layer with $l=4$. On the contrary, the amplitudes of the Nb–O and K–O displacement (except $l=6$) for the P_- state are all smaller than bulk values. Obviously, compared to bulk KNbO₃, the ferroelectricity of the KNbO₃ barrier in the P_+ and P_- states is enhanced and reduced, respectively. An unusual situation appears at the KO termination. We can find that the K–O displacements at the right interface for the P_+ and P_- states are -0.21 and $-0.33 \text{ \AA}$ respectively. The sign of the K–O displacements does not change when the polarization reserves. This is strange since the sign of the

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