Enhanced thermal spin transfer in MgO-based double-barrier tunnel junctions

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Abstract

Based on atomic first principles, we predict enhanced thermal spin transfer (TST) effects and small switching temperature gradient in Fe|MgO|Fe|MgO|Fe double-barrier magnetic tunnel junctions (MTJs). At room temperature, temperature gradient \(\Delta T \approx 10\,\text{K}\) with \(\nabla T \approx 10\,\text{K}\,\text{nm}^{-1}\) across barriers would be sufficient to switch the magnetic configurations circularly in a junction with 3 MgO atomic layers (L), which is about one order smaller than that in Fe|MgO(3L)|Fe MTJs. This temperature gradient is under the current experimental capability. The resonant quantum-well states in companion with resonant interfacial states are responsible for the enhancement. Moreover, a thermal induced ‘off’ state is found in a double-barrier MTJ.

1. Introduction

Switching the magnetic order parameter thermally is the basis for spin caloritronic applications such as logic devices and memories [1]. As a easy, efficient, and ‘green’ method to manipulate the magnetic order parameter, thermal spin transfer (TST) torque has received much attention recently [1–14]. To achieve TST torque (also called thermal torque) comparable to that induced by an electric bias, a large temperature gradient across magnetic elements should be established. Marked TST effect is first reported in a MgO-based magnetic tunnel junctions (MTJs) with ultra-thin barrier [2, 3]. Therein, the skewed TST torque is more favorable to magnetic oscillation rather than switching, a temperature gradient \(\Delta T \approx 60\,\text{K}\) with \(\nabla T \approx 100\,\text{K}\,\text{nm}^{-1}\) is predicted to be needed to switch the magnetic configurations circularly, which is beyond the current experimental capability. The steady-state temperature gradient in MTJs is relatively small, a temperature gradient \(\Delta T \approx 20\,\text{K}\) with \(\nabla T \approx 32\,\text{K}\,\text{nm}^{-1}\) with order of ten picoseconds can be established by femtosecond laser pulses heating [4]. Thus, seeking materials with moderate switching temperature gradient is an urgent and important task in spin caloritronics.

It is resonant interfacial states, widely existed in high quality nanostructures, that to be responsible for the large TST in MgO-based MTJs [3]. Similar to interfacial states, quantum-well (QW) states can lead to resonant tunneling [15–18] and large spin transfer effects. QW states can be engineered easily by the structure parameters such as thickness and materials of barrier and spacer metal, crystal defects and so on [16–19]. Spin transfer torque created by bias voltage in double-barrier MTJs (DBMTJs) is well studied [20–27]. When the QW states calibrate to Fermi energy \((E_F)\), thermoelectric effects, including TST, would be enhanced. In DBMTJs, both the resonant QW states and interfacial states can be coexistent. So, larger TST effect and a smaller temperature gradient for magnetic switching would be expected in DBMTJs than those in single-barrier MTJs (SBMTJs). However, as far as we know, few works on this subject have been reported both in experiments and theory.

In this work, we focus on the TST torque in MgO-based DBMTJs in the presence of nonequilibrium thermal distribution by applying the Landauer–Büttiker formalism with thermal bias [3]. We consider an ultra-
thin MgO barrier with thickness of three atomic layers (about 0.6 nm) as spin transfer torque (STT) decrease exponentially as barrier thickness increases [5]. Our results show enhanced STT torque in DBMTJs owing to the coexistence of the resonant QW states and the resonant interfacial states. Based on Landau–Lifshitz–Gilbert (LLG) equation, [28] we estimate that a temperature gradient of 10 K nm⁻¹ across barriers would be sufficient to reverse the magnetic configurations circularly at room temperature.

This paper is organized as follows. In section 2, we give the details of our calculation based on first-principle scattering theory. In section 3, we present our results on Fe | MgO | Fe | MgO | Fe DBMTJs with clean and disordered interfaces. Section 4 is our summary.

2. Electronic structure and transport calculations

Considering a DBMTJ as sketched in the inset of figure 1 with temperature and voltage bias across the barriers, the local thermal equilibrium can be depicted by Fermi–Dirac distribution function $f_{L/R}(\epsilon) = e^{(\epsilon - \mu_{L/R})/k_B T_{L/R}} + 1)^{-1}$ and local chemical potentials $\mu_{L/R}$ and temperatures $T_{L/R}$. TST torque transferred to the magnetization $M$ can be estimated by the spin current pumped out of the precessing $M$ based on scattering theory [30]

$$ T^T = \frac{\Delta TM JV}{eT_0} \sum_{k,j} \int dE \frac{\partial f}{\partial E} [m_j^j \times (\text{Tr} [Q(k, E)] \times m_j^i)], \quad (1) $$

where $Q(k, E) = Q^L(k, E) - Q^R(k, E)$ with $Q_{L/R}^j = \frac{ie}{4\pi M_j V} \sum_{S_L/S_R} S_0 S_j^i S_j^i + H.c$ sums all modes over left/right (L/R) lead and $S_k(E)$ is the scattering matrix that is evaluated at the energy $E$ and $k$ in the two-dimensional Brillouin zone (2D BZ). $m$ and $m_j^i$ are the unit vector along $M$ and $M_j^i$ with respect to saturation magnetization $M$ in ferromagnetic region with volume $V$, $T_0 = (T_L + T_R)/2$ is ambient temperature, and $\Delta T = T_R - T_L$ is temperature bias. Therein, the magnetization dependent parameter $Q$ is the key to equation (1), which is well-studied by spin pumping theory [31, 32]. By putting TST torque into the phenomenological LLG equation [2], one can estimate thermal induced magnetic dynamics.

We consider two stable DBMTJ structures as shown in figure 1. Therein, S1/S2 has one/two magnetization fixed along z quantum axis and two/one free magnetizations, and the magnetic structure of S1 is similar to SBMTJs. In calculations, we neglect the minor lattice mismatch at Fe | MgO interface and fix the interfacial atoms at their bulk positions. For disordered interface, we assume oxygen vacancies (OV) only exist at the first layer of MgO attached to Fe. In the transport calculations, an $800 \times 800$ k-mesh is used to sample the two-dimensional Brillouin zone (2D BZ) to ensure good numerical convergence. More numerical details of the electronic structure and transport calculations can be found elsewhere [3, 33]. To check the validity of

![Figure 1. Thermal torque in clean Fe | MgO(3)| Fe(8)| MgO(3)| Fe DBMTJs at room temperature. Lower inset: the ratio of the in-plane TST torque to thermocurrent ($T^T / I^T$). Upper inset: schematic structure of the Fe | MgO | Fe | MgO | Fe DBMTJs. We consider a temperature bias $\Delta T = T_R - T_L$ and voltage bias $V_S = V_L - V_R$ across barriers, and set temperature bias drop within barriers as estimation in [29]. We consider two representable configurations here. S1: the magnetization of the left lead $M_L$ is fixed along $z$ quantum axis, and both the magnetization of sandwiched Fe $M$ and right lead $M_R$ are set free with relative angle $\theta$ to $M_L$. S2: $M_L/M_R$ is fixed along $+z$ – $z$ quantum axis, and $M$ is set free.](image-url)
Table 1. Thermal torque in clean and dirty (in brackets) Fe [MgO(3)] Fe(8) MgO(3)] Fe DBMTJs at $T = 300$ K and $\Delta T = 1$ K for $\theta = 90^\circ$. For dirty case, we consider 4% OV at Fe [MgO] interfaces of right side MgO barrier.

| FM Structure | TMR (%) | $T_T^2$ (nJ m$^{-2}$ K$^{-1}$) | $\Lambda$ | $\Delta T_{SW}$ (K) | $\nabla T_{SW}$ (K nm$^{-1}$) |
|--------------|---------|-------------------------------|--------|---------------------|-----------------------------|
| Fe S1        | 1540    | $-220$                        | 1.5    | 19                  | 16                          |
| FeCo S1      | 860     | $-125$                        | 1.0    | 25                  | 21                          |
| Fe S2        | 0(110)  | $-370(-270)$                  | 1.0(1.0)| 9(12)              | 7.5(10)                     |
| FeCo S2      | 110     | $-220$                        | 1.0    | 14                  | 12                          |
| Fe [MgO(3)] Fe | 1300(200)| $-195(-110)$             | 3.5(1.5)| 45(33)             | 75(55)                      |
| Fe [MgO(3)] FeCo | 420  | $-40$                        | 1.0    | 76                  | 126                         |

3. Thermal torque in Fe [MgO] Fe [MgO] Fe DBMTJs

Figure 1 shows the angular dependence of the in-plane TST torque ($T_T^2$) in clean Fe [MgO(3)] Fe(8) MgO(3)] Fe DBMTJs. Theret, $T_T^2$ in S2 is symmetric with parameter $\Lambda = 1.0$ with peak value of $-370$ nJ m$^{-2}$ K$^{-1}$ at $\theta = 90^\circ$, while that in S1 is asymmetric ($\Lambda = 1.5$) with peak value of $-230$ nJ m$^{-2}$ K$^{-1}$ at $\theta = 120^\circ$. The former is nearly double larger than the latter. However, both $T_T^2$ in S1 and S2 structures are larger than that $(-195$ nJ m$^{-2}$ K$^{-1}$ at $\theta = 90^\circ$) in clean Fe [MgO(3)] Fe SBMTJs. At the same time, $\Lambda$ in both S1 and S2 are smaller than that 3.5 in clean Fe [MgO(3)] Fe SBMTJs. It is rather interesting because the larger $T_T^2$ companied with smaller $\Lambda$ would favor the magnetization switching in DBMTJs than SBMTJs [2]. The out-of-plane part of TST torque ($T_T^3$) is about 10% of $T_T^2$, and we neglect $T_T^3$ in magnetic dynamic simulations. By putting TST torque into LLG equation [28], we get temperature gradient $\Delta T_{SW} = 19/9$ K ($\Delta T_{SW} = \max (\Delta T_{SW}^{AP}, \Delta T_{SW}^{AP-P})$) and $\nabla T_{SW} = 16/7.5$ K nm$^{-1}$ to switch between antiparallel (AP) and parallel (P) configurations in S1/S2 structure as shown in table 1, which is considerably smaller than that in SBMTJs with same barrier thickness.

To check the parameters used in magnetic dynamics simulations, we estimate $\Delta T_{SW} \approx 16.4$ K in clean Fe [MgO(3)] Fe(8) MgO(3)] Fe SBMTJs with S1 structure by taking experimental data, which shows minor difference (~10%) from that obtained from LLG calculations. So, we conclude that the parameters in magnetic dynamic simulations are reasonable.

Huge ratio of the TST torque to thermocurrent $T_T^2/T_T^1$ in S1 and S2 structures is found in a large energy range, as shown in the lower inset in figure 1. A saturated $T_T^2/T_T^1 \approx 300$ h/2e is found at $\theta = 75(105)^\circ$ in S2 structure. For S1 structure, $T_T^2/T_T^1 \rightarrow \infty$ at $\theta \approx 116^\circ$ as $T_T^1 \rightarrow 0$, this is a ‘off’ state produced thermally. The small thermocurrent $T_T^1 = \frac{\Delta T}{T} \int [dE (E - E_f) T(E) \frac{d\rho}{dE}]$ is responsible to the huge $T_T^2/T_T^1$ here, where $T(E) = Tr [tr^t]$ is electronic transmission and $r$ is the transmission part of the scattering matrix. The small $T_T^1$ can be understood from the small asymmetry in electronic transmission within thermal energy window $k_B T_{SW}$ at room temperature, as shown in the upper inset of figure 2(a). The giant spin transfer efficiency in DBMTJs would favor the functional of devices. Furthermore, the ‘off’ state demonstrated here can be found logic device application.

To check the source of the enhancement of TST torque in clean Fe [MgO(3)] Fe(8)] MgO(3)] Fe DBMTJs, we check the energy-dependent voltage torkance

$$\tau_T(E) = \mu L V \sum_{ij} m_i \times (Tr Q(k, E)) \times m_j$$

4. Noackowski proposed a symmetric parameter $\Lambda = G / \sqrt{G_1 G_2}$ for angular dependent torques with conductance $G_i = -e^2/h \int dE \langle T(E) \rangle^{\partial^2} / dE$ with $T$ is the transmission part of the scatter matrix $S$ and $G = G_1 + G_2$. The parameter would be invalid in case such as 100% spin polarization. In the calculations, we estimate the parameter by supposing the torques following the relation: $\tau_T(E) / \tau_T(\theta = 2) = (\Lambda \cos^2 (\theta / 2) + \sin^2 (\theta / 2)) / \Lambda / \Lambda^2$.

5. In a recent experiment, $STT / \sin(\theta) \approx 8.2 / 20 \mu$ Tm$^{-1}$ is needed to switch a 3.9 nm CoFe magnetization from P/AP to AP/P configurations. For clean Fe [MgO(3)] Fe(8)] MgO(3)] Fe DBMTJs with S1 structure, $T_T^{SW-AP}$ $\approx 16.4$ K and $T_T^{SW-AP-P}$ $\approx 10.5$ K is needed to switch a 12 nm magnetization.
with \( \mathbf{M} \) and \( \mathbf{M}_{L/R} \) perpendicular to each other. For S1 structure, \( \mathbf{M}_{L} \) is along the \( z \) axis while \( \mathbf{M} \) and \( \mathbf{M}_{R} \) is parallel to the \( x \) axis. For S2 structure, \( \mathbf{M}_{L} / \mathbf{M}_{R} \) is along \( z - z \) while \( \mathbf{M} \) is parallel to \( x \). The processing \( \mathbf{M} \) would pump spin current into both left and right leads, the left-going and right-going spin current are equal for S2 structure, while only left-going spin current existed in S1 structure. When \( \mathbf{M} \) rotates towards the \( x / y \) direction, a in-plane/out-of-plane torkance \( (\tau^{v}_{x/y}) \) will be produced. We plot the results in figure 2(a) in the energy range \( [E_{F} - 0.4 \text{ eV}, E_{F} + 0.4 \text{ eV}] \). Therein, \( \tau^{v}_{x/y} \) show a striking negative peak with value of \(-120 / -250 \times 10^{-14} \) \( \tau_{0} \equiv \hbar k (\Omega^{-1}\text{m}^{-2}) \) at \( E_{F} - 0.07 \text{ eV} \) and a broaden positive peak with value of \( 80 / 130 \times 10^{-14} \tau_{0} \) at \( E_{F} + 0.02 / E_{F} + 0.06 \text{ eV} \) in S1/S2 structure. At both peaks, \( \tau^{v}_{x/y} \) in S2 structure is almost double larger than that in S1 structure due to the double spin transfer process existed in S2 structure, as expressed in equation (2). Both the two peaks contribute to room temperature TST torque. We take S1 structure as an example to analyze the \( k \)-resolved contribution to \( \tau^{v}_{x/y} \). Figure 2(b) plot the \( k \)-resolved \( \tau^{v}_{x/y} \) at \( E_{F} - 0.07 \text{ eV} \) and \( E_{F} + 0.07 \text{ eV} \). The former is dominated by several bright spots in \( \downarrow \) spin, while the latter is dominated by a bright ring in \( \uparrow \) spin.

The out-of-plane torkance \( \tau^{v}_{z} \) in DBMTJs shows complicate energy dependency as shown in the lower inset of figure 2(a). Although the out-of-plane TST torques in both S1 and S2 structures are relatively small, the out-of-plane voltage torque are rather considerable. We observe large ratio \( \tau^{v}_{z} / \tau^{v}_{x/y} = 3.0 / 0.9 \) at \( E_{F} \) in S1/S2 structure, which is considerable larger than that (\(~0.25\) at \( E_{F} \)) in Fe\( \mid \text{MgO}(3) \mid Fe \) SBMTJs.

DBMTJ can be considered as two SBMTJs connected in series. The coupling between SBMTJs in DBMTJ can be estimated from the electron transmission. When the electron transmission in DBMTJ \( (T_{d}) \) and SBMTJs \( (T_{i}) \) follow/beyond the relation \( T_{d} = T_{i} \ast T_{i} \), the coupling of SMJTs in DBMTJs would be weak/Strong. For clean Fe\( \mid \text{MgO}(3) \mid Fe \) SBMTJs with S1/S2 structure, \( T_{d} \) is 0.012 / 0.013 at \( E_{F} \), which is close to that.
\(T_r = 0.02\) in Fe | MgO(3)| Fe MTJs, indicating strong coupling between SBMTJs. It is noted that the resonant interfacial states in \(d\) spin and resonant QW states in \(s\) spin that should be responsible to the strong coupling. From the value of \(T_d\) and \(T_a\), we estimate that the resonant states would contribute to \(\sim 50\%\) of \(T_d\) in DBMTJs at \(E_F\). Moreover, STT can be used to estimate the coupling of SBMTJs in DBMTJ also, which is related with electron transmission by a simple relation [37].

Due to the strong coupling between SBMTJs in DBMTJ, the energy-dependent torkances for \(k_x a_0 = 1.03\) and \(k_y a_0 = 1.67\) at \(E_F - 0.07\) eV (point A in figure 2(b)) produce three resonant peaks as shown in figure 2(c), which is different from the double peaks scheme in SBMTJs. The energy-dependent torkance share the same shape as the electronic transmission, indicating that the resonant peaks are from interfacial states. Differently, the energy-dependent torkance for \(k_x a_0 = 0.4\) and \(k_y a_0 = 0.0\) at \(E_F + 0.07\) eV (point B in figure 2(b)) give a large resonant peak and two ghost peaks, as shown in figure 2(d). The former is from the resonant QW states, and the latter is from the resonant interfacial states.

Both the resonant interfacial and QW states contribute to the TST torque in DBMTJs. The position of resonant QW states is sensitive to the thickness of sandwich metal, while the position of resonant interfacial states is stable. Figure 3 shows the contribution of resonant interfacial and QW states to the TST torque in clean Fe | MgO(3)| Fe | MgO(3)| Fe DBMTJs with respect to the thickness of the sandwiched Fe. Therein, the TST torque in junction with S1/S2 structure increases quickly as \(n\) increases, and reaches a saturation value \(\sim \sim 210 / \sim \sim 410\) nJ m\(^{-2}\)K\(^{-1}\) for \(n = 12\). In addition, the contribution from resonant interfacial states saturate at a value \(\sim -130 / \sim -260\) nJ m\(^{-2}\)K\(^{-1}\) for \(n \geq 12\), and the contribution from resonant QW states show a convex curve with peak value of \(\sim -110 / \sim -190\) nJ m\(^{-2}\) for \(n = 8\).

Owing to the presence of the double spin transfer process, DBMTJs with S2 structure show large TST torque with symmetric angular-dependency, which would favor thermal induced magnetic switching. However, symmetric DBMTJs with S2 structure show zero tunnel magnetoresistance (TMR = \((G(0) - G(\pi))/G(\pi)\) with conductance \(G(E) = (e^2/h) T(E)\). To achieve observable TMR and large TST at the same time, asymmetric DBMTJs with S2 structure can be devised. Here, we pay attention to the effects of asymmetric interfacial OV and asymmetric leads on \(\tau^{\text{eff}}_d\) in DBMTJs with S2 structure, as shown in figure 4 and table 1. Firstly, we study the asymmetric interfacial OV, where the Fe | MgO interfaces of left MgO barrier keep clean while that of right MgO barrier is dirty. We find that 4% OV at Fe | MgO interfaces of right side MgO can produce TMR \(\sim 110\%\) at zero bias, simultaneously \(\tau^{\text{eff}}_d\) decreases to \(-270\) nJ m\(^{-2}\)K\(^{-1}\), as shown in table 1. Detail study shows interfacial OV would deteriorate both resonant interfacial and QW states. The resonant interfacial states are more sensitive to OV than the QW ones, as shown in figure 4. Quantitatively, \(\tau^{\text{eff}}_d\) from resonant interfacial/QW states at energy \(E_F - 0.07/E_F + 0.05\) eV is \(-140/100 \times 10^{14}\tau_0\), show a reduction of 60/20 comparing with that in the clean structure. The asymmetric interfacial OV does not change the symmetry of the angular-dependency of the TST torque, and \(\Delta T_{SW} \sim 12\) K with \(\nabla T_{SW} \sim 10\) K nm\(^{-1}\) are estimated according to the LLG simulation.

When the bcc-Co\(_{0.5}\)Fe\(_{0.5}\) alloy is used as the right lead, the resonant interfacial states would be quenched completely, while resonant QW states keep stable. The clean asymmetric Fe | MgO(3)| Fe(8)| MgO(3)| FeCo...
DBMTJs with S2 structure show TMR $\sim 110\%$ at zero bias and symmetric angular-dependent TST torque with peak value of $-220 \text{ nJ m}^{-2} \text{ K}^{-1}$ at $\theta = 90^\circ$, and $\Delta T_{SW} \sim 14 \text{ K}$ with $\nabla T_{SW} \sim 12 \text{ K nm}^{-1}$ are estimated from the magnetic dynamic simulation.

In table 1, we summarize the TST torque in Fe $|$ MgO $|$ Fe $|$ MgO $|$ Fe DBMTJs. Therein, DBMTJs with SBMTJ-like magnetic structure (S1) show larger TMR, while those with S2 structure show larger TST torque. By introducing asymmetric OV or asymmetric leads, DBMTJs with S2 structure can give considerable TMR and larger TST torque. $D_{T \sim T_{SW}}$ with $\nabla T_{SW} \sim 10 \text{ K nm}^{-1}$ is presented in an asymmetric DBMTJs with S2 structure, which is about one order smaller than that in SBMTJ with same barrier thickness. For same TST torque, the ratio of $D_{T \sim T_{SW}}$ and $\nabla T_{SW}$ in SBMTJs to those in DBMTJs is $\Lambda$ and $2.0 \times \Lambda$, respectively.

Furthermore, when 4% OV is introduced in Fe $|$ MgO $|$ Fe MTJs, the effect of the reduction in $\Delta T_{SW}$ cancel that of the reduction in TST torque, leading to smaller $D_{T \sim T_{SW}}$ and $\nabla T_{SW}$ comparing with clean junctions, as shown in table 1. It is suggested that, crystal defects such as interfacial OV, may be not always a deleterious factor to magnetic switching.

Owing to the involvement of resonant QW states, TST torque in DBMTJs is enhanced. At the same time, the angular-dependency of TST torque gets symmetric or close to symmetric. Both factors lead to considerable reduction in $\Delta T_{SW}$ and $\nabla T_{SW}$ comparing with the SBMTJs with the same barrier thickness. So, we predict that MgO-based DBMTJs is more promising in application for thermally induced magnetization switching.

4. Summary

We predict enhanced TST torque and small switching temperature gradient in Fe $|$ MgO $|$ Fe $|$ MgO $|$ Fe DBMTJs from atomic first principles. Temperature gradient $\Delta T_{SW} \sim 10 \text{ K}$ with $\nabla T_{SW} \sim 10 \text{ K nm}$ across MgO barriers is predicted to drive the magnetic configurations in a DBMTJs switch circularly at room temperature, which is about one order smaller than that in Fe $|$ MgO $|$ Fe MTJs, and under the current experimental capacity. The coexistence of resonant QW states and resonant interfacial states is responsible to the enhancement. The introduction of asymmetry by interfacial OV and different leads would change TMR and TST torque including their angular dependency. Moreover, zero thermocurrent can present at a specific angle in a DBMTJ, indicates that we can produce a ‘off’ state in the material thermally. Based on these results, we predict that MgO-based DBMTJs is promising in application for heat-flow-induced magnetization switching and logic device.

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