Ab initio studies of the spin-transfer torque in tunnel junctions

Christian Heiliger\textsuperscript{1,2} and M. D. Stiles\textsuperscript{1}

\textsuperscript{1}Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD 20899-6202
\textsuperscript{2}Maryland NanoCenter, University of Maryland, College Park, MD, 20742

(Dated: February 2, 2008)

We calculate the spin-transfer torque in Fe/MgO/Fe tunnel junctions and compare the results to those for all-metallic junctions. We show that the spin-transfer torque is interfacial in the ferromagnetic layer to a greater degree than in all-metallic junctions. This result originates in the half metallic behavior of Fe for the $\Delta_1$ states at the Brillouin zone center; in contrast to all-metallic structures, dephasing does not play an important role. We further show that it is possible to get a component of the torque that is out of the plane of the magnetizations and that is linear in the bias. However, observation of such a torque requires highly ideal samples. In samples with typical interfacial roughness, the torque is similar to that in all-metallic multilayers, although for different reasons.

PACS numbers: 73.63.-b, 75.70.Cn, 75.30.Et, 71.15.Mb

The discovery of giant magnetoresistance (GMR) in spin-valve systems\textsuperscript{1,2} and the rediscovery of the tunneling magnetoresistance (TMR) in tunnel junctions\textsuperscript{3,4} has led to applications such as hard-disk read heads, sensors, and storage elements in magnetic random access memory (MRAM). Both GMR and TMR occur in junctions in which two ferromagnetic leads are separated by a spacer layer, which is a non-magnetic metal in case of a GMR junction and a tunnel barrier for a TMR junction. The resistance $R$ and therefore the conductance $g$ of these junctions are a function of the relative angle $\theta$ between the magnetizations of the ferromagnetic leads. The magnetoresistance (MR) ratio is $[R(180^\circ) - R(0^\circ)]/R(0^\circ)$. Typical GMR ratios are in the range of 50\%\textsuperscript{5} and can be explained by spin dependent interface scattering in a semiclassical picture\textsuperscript{6,7,8}. TMR ratios can exceed several hundred percent in crystalline Fe/MgO/Fe tunnel junctions\textsuperscript{9,10} as predicted theoretically\textsuperscript{11,12}.

These high TMR values in crystalline Fe/MgO/Fe junctions originate in the symmetry-dependent transmission probabilities through the MgO barrier at the Brillouin zone center ($\Gamma$ point) combined with the exchange splitting of the Fe band structure\textsuperscript{5,11}. States which have the full rotational symmetry of the interface, said to have $\Delta_1$ symmetry, decay the most slowly in MgO and hence dominate the tunneling current. At the Fermi level, Fe is a half metal at the $\Gamma$ point for states with $\Delta_1$ symmetry, having only majority states. The half metallic nature of the states that dominate the tunneling leads to a much higher current for parallel than for antiparallel alignment of the magnetizations.

Spin-transfer torque, an effect predicted by Slonczewski\textsuperscript{13,14} and Berger\textsuperscript{15}, can be used to switch the magnetic orientation of ferromagnetic layers in GMR and TMR devices. For this purpose a current is driven through the sample and becomes spin polarized in one ferromagnetic layer. This polarization persists going through the spacer layer and entering the other ferromagnetic layer. If the spins of the polarized current are not aligned with the magnetization, they precess around it. This precession in turn creates a torque on the magnetization and can reverse the magnetization if the current is high enough. There is currently significant interest in understanding spin-transfer torques in tunnel junctions as a way to allow the development of MRAM applications\textsuperscript{14}.

Spin transfer torques are well understood in all-metallic trilayer structures\textsuperscript{17}. There, the current is carried by electrons over the whole Fermi surface. In ferromagnetic layers and at their interfaces, electrons precess at different rates and the components of the spins transverse to the magnetization rapidly become out of phase from each other. Two properties of the torque follow from the strong dephasing of the electron spins\textsuperscript{18}. First, the spin transfer torque largely occurs at the interfaces between ferromagnetic layers and non-magnetic layers. Second, it is largely in the plane defined by the magnetizations of the two ferromagnetic layers. These properties are used in almost all modelling of dynamics of GMR devices\textsuperscript{14} and have been used without change in the modelling of TMR devices.

In typical tunnel junctions, the current and spin current are carried by a small fraction of the Fermi surface and dephasing is greatly reduced. Here, we use ab initio calculations to compute the spin transfer torques in Fe/MgO/Fe tunnel junctions. We show that in spite of the reduced dephasing, the torque is still approximately confined to the interface and the in-plane torque is much larger than the out-of-plane torque (see Fig.\textsuperscript{11}).

We treat the same structure as in previous studies on Fe/MgO/Fe\textsuperscript{19} taking into account the experimentally observed relaxation of the Fe layer next to the interface\textsuperscript{20}. The junctions consist of an Fe fixed layer, an MgO barrier, and an Fe free layer embedded between semi-infinite Cu in a bcc-Fe structure. The potentials are calculated self-consistently using a screened Korringa
Kohn Rostoker multiple scattering Green’s function approach. We obtain potentials for junctions with different free layer thicknesses using the frozen potential approximation and the potentials from a calculation with 20 Fe monolayers in each magnetic layer. We calculate the linear-response torque using the magnetic moment \( \delta \vec{m}(E_F) \) of those electrons that contribute to the current. The torque \( d\vec{\tau}/dV \) is the variation of the torque \( \vec{\tau} \) with the voltage \( V \). The torque acting on layer \( i \) is \[ d\tau_i/dV = \frac{\mu_B g_0}{2eA} \tilde{\Delta}_i \times \delta \vec{m}(E_F), \] where \( \tilde{\Delta} \) is the exchange field pointing in the direction of the magnetization of the corresponding layer, \( A \) is the area of the in-plane unit cell, and \( g_0 = e^2/h \) is the quantum of conductance. For a description of our implementation of the non-equilibrium Green’s function technique see Refs. 21, 22, 23. The total non-equilibrium magnetization \( \delta \vec{m}_{\text{tot}}(E_F) = (1/2)[\delta \vec{m}^L(E_F) - \delta \vec{m}^R(E_F)] \) contains separate contributions from electrons incident from the left and holes incident from right (for a positive bias).

Fig. 2 shows our ab initio calculations of the torque as a function of the relative angle \( \theta \) between \( \vec{M}_L \) and \( \vec{M}_R \) for different thicknesses of the free layer. Both the component in the plane of the two magnetizations, \( d\tau_{||}/dV \), and the component out of the plane \( d\tau_{\perp}/dV \) are almost perfectly sinusoidal. For current biased applications, the torque per current \( d\vec{\tau}/dI \) is of greater interest. This is related to the torque by the conductivity \( g = dI/dV \), \( g(d\vec{\tau}/dI) = d\vec{\tau}/dV \). In tunnel junctions with very high TMR ratios the conductivity depends strongly on the angle between the magnetizations so that \( d\vec{\tau}/dI \) is highly asymmetric. The critical voltages and currents for switching out of the parallel and antiparallel states are proportional to the inverses of the slopes of these curves at \( \theta = 0^\circ \) and \( 180^\circ \) respectively.

The bottom left panel of Fig. 2 shows that both the in-plane and out-of-plane torque oscillate as a function of the Fe free layer thickness. The oscillations fit a sine curve with a period that is incommensurate with the lattice spacing (hence the apparent beating of the amplitude). This period is very close to the Fermi wave vector of the \( \Delta_1 \) band in Fe at the \( \Gamma \) point. This agreement of the periods indicates that the important states are located close to the Brillouin zone center. The conductance shows similar oscillations 19, so that the torque per current in the right bottom panel of Fig. 2 is largely independent of the thickness. However, there is a phase shift between the oscillations in the in-plane and out-of-plane torque so that the oscillations in \( d\tau_{\perp}/dI \) are even stronger than they are in the torque.

Similar oscillations of the conductance and magnetoresistance have been observed as a function of the thickness of an additional nonmagnetic layer inserted next to the barrier 24, 25. For Fe/MgO/Fe, the origin of these oscillations is subtle. As we show below, the torque is largely restricted to the interface because the minority component is evanescent. However, the torque changes as a function of the free layer thickness due to coherent effects: specifically, phase shifts in the majority channel due to quantum well states.

Note that in Fig. 2 the torque per current is very close to \( \mu_B/e \) when the magnetizations are at an angle of 90°. This is the expected behavior for a simple model of a junction between two half metals, for which the polarization of the current is 100%. Each electron spin that traverses the junction rotates by 90°. This change in angular momentum is shared by the fixed and free layers. Since the torque must be perpendicular to the magnetizations, the change in angular momentum supplied to each layer must be \( \mu_B \). For greater angles, the torque per current can be several factors higher, a result that seems counterintuitive. In fact, as the barrier is made
Consider a free layer with a magnetization at a relative orientation of either 45° or 135° with respect to that of the fixed layer. In both cases, the majority electrons that tunnel from the fixed layer have the same transverse component and will exert roughly the same torque. The electrons tunneling into the free layer with a magnetization at 45° are approximately 85% majority and 15% minority in the free layer while the electrons tunneling into the free layer with a magnetization at 135° are approximately 15% majority and 85% minority in the free layer. The tunneling current will be much greater in the former case than in the latter so that the ratio of the torque to the tunneling current will be greater when the layers are at 135°.

The weak influence of free layer thickness on $d\tau_\perp/dI$ in Fe/MgO/Fe and the saturation for more than three monolayers of Fe implies that the torque is restricted to the layers next to the interface even though there is only minimal dephasing. To understand this behavior, the right panel of Fig. 3 shows our ab initio results for the layer resolved torque. We analyze this result by comparison to a simple free electron model in the left panel of Fig. 3.

In the simple model, we use the wave vectors of the $\Delta_1$ band in Fe at the Fermi level to model the half metallic nature at the $\Gamma$ point. In a half metal, the components of the non-equilibrium magnetization perpendicular to the magnetization and hence the torque arise from coherent interference between the majority and minority spin components. Since the minority state is evanescent, the torque must decay. After a short distance only the component of the spin current pointing along $\hat{M}_R$ is left. The decay of the torque, which results from the half-metallic character of the ferromagnetic electrodes, is even faster than in spin-valve systems where the decay follows a power law resulting from dephasing [18]. The agreement between the ab initio results and the simple model emphasizes that the states around the Brillouin zone center dominate the torque within the free layer.

During this decay, the electrons precess around $\hat{M}_R$ within the $zy$ plane leading to decaying oscillations of the components of the magnetic moments of the conduction electrons along the $z$ and $y$ directions. These oscillations in the magnetic moments are phase-shifted by 90° with respect to each other [20]. They lead to the oscillations in the torque components having the corresponding phase shift as discussed in Fig. 2. Within a given layer, the sizes of $\tau_\parallel$ and $\tau_\perp$ are comparable on average. The total torques are determined by the starting phase and the strength of the decay. In addition, Fig. 3 only shows the torque of right-going electrons. The contributions of left-going holes have to be added in order to obtain the torque in Eq. 1.

There are additional contributions to the torque that are important for thinner barriers but are negligible for 6 monolayer and thicker barriers. In Fig. 2 there are oscillations that are barely visible, which originate in states away from the Brillouin zone center for which Fe is not half-metallic. These oscillations are long ranged due to reduced dephasing and could be important for barriers that are thinner than those typically fabricated.

Our calculations of the bias dependence of the out-of-plane component of the torque address a topic of recent experimental interest. Spin-transfer-driven ferromagnetic resonance (ST-FMR) quantitatively measures the magnitude and direction of the spin transfer torque in tunnel junctions [27, 28, 29]. Tulapurkar et al. [27] measured a linear dependence of $\tau_\perp$ on the applied bias for small voltages (non-zero $d\tau_\perp/dV$) whereas Sankey et al. [30] measured $\tau_\perp$ to be linearly independent of $V$.

This latter result is consistent with theoretical arguments [31, 32] that hold in special cases. For junctions that are symmetric about the center of the barrier and in which electrons leaving the ferromagnetic layers into the leads are aligned with the magnetizations, the left going electrons cause the same out-of-plane torque in the free layer as the right going ones, that is $\tau_\perp(E_F) = \tau_\perp^R(E_F)$. When the outgoing electrons are aligned with the magnetizations, the total torque on both layers in a symmetric junction must be in-plane. If this condition holds, Eq. 1 gives $d\tau_\perp/dV = 0$ and there is no linear dependence on the applied voltage for small biases. However, for asymmetric junctions these arguments do not apply.

Figure 2 shows that it is possible to get a significant out-of-plane component of the torque in tunnel junctions that are close to ideal. However, thickness fluctua-
tions in a real junctions lead to an averaged torkance. To simulate such fluctuations we assume the structure shown in the left panel of Fig. 4. The right panel shows the corresponding averaged torkance. Comparing to Fig. 2 shows two consequences of the thickness fluctuations. First, the oscillation of the in-plane component vanishes and second, the out-of-plane component itself vanishes. This behavior is consistent with the experimental results in Ref. 30. Therefore, to actually measure a non-vanishing out-of-plane component of the torkance or an oscillating behavior of the in-plane component requires samples that are close to ideal. For most samples the out-of-plane component will vanish.

In conclusion, we show that the spin-transfer torque in Fe/MgO/Fe tunnel junctions behaves very similarly to the behavior found in all-metallic devices. The spin transfer torque is largely localized to the interfaces and largely in the plane defined by the two magnetizations. The dominant contribution to the tunneling and the dephasing. For a perfect sample we expect some small out-of-plane component and an oscillation of the in-plane component of the torkance as a function of the free layer thickness. However, small fluctuations of the thickness will average out this component.

This work has been supported in part by the NIST-CNST/UMD-NanoCenter Cooperative Agreement. We thank Dan Ralph and Paul Haney for useful conversations.

* Electronic address: christian.heiliger@nist.gov

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