Ab Initio Studies of the Spin-Transfer Torque in Magnetic Tunnel Junctions

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We calculate the spin-transfer torque in Fe/MgO/Fe tunnel junctions and compare the results with those for all-metallic junctions. The spin-transfer torque is interfacial due to the half-metallic nature of the Fe Δ_1 states. For samples with typical interfacial roughness, the in-plane torque varies linearly with bias and the out-of-plane torque varies quadratically, both in quantitative agreement with experiment. For ideal samples, we predict that the out-of-plane component of the torque varies linearly with bias and oscillates as a function of the ferromagnetic layer thickness.

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The discovery of giant magnetoresistance (GMR) in spin-valve systems [1,2] and the rediscovery of the tunneling magnetoresistance (TMR) in tunnel junctions [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 nonmagnetic metal in the 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 θ between the magnetizations of the ferromagnetic leads. The magnetoresistance ratio is $[R(180°) - R(0°)]/R(0°)$. Typical GMR ratios are in the range of 50% [5] and can be explained by spin-dependent interface scattering in a semiclassical picture [6–8]. TMR ratios can exceed several hundred percent in crystalline Fe/MgO/Fe tunnel junctions [9,10] as predicted theoretically [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 ($\bar{\Gamma}$ point) combined with the exchange splitting of the Fe band structure [5,11]. States which have the full rotational symmetry of the interface, said to have Δ_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 $\bar{\Gamma}$ point for states with Δ_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 torques, predicted by Slonczewski [13,14] and Berger [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 creates a torque on the magnetization and can reverse the magnetization if the current is high enough. There is currently significant interest in spin-transfer torques in tunnel junctions as a way to advance the development of MRAM applications [16]. The critical current necessary to switch the magnetization is of crucial importance to these applications. The critical current depends on the current-induced torque, the topic of the present Letter, but also on details such as the sample shape and any anisotropies that are present.

Spin-transfer torques are well understood in all-metallic trilayer structures [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. The strong dephasing of the electron spins has two consequences [18]. First, the spin-transfer torque largely occurs at the interfaces. Second, it is largely in the plane defined by the magnetizations of the two ferromagnetic layers. These properties are used in almost all modeling of dynamics of GMR devices [17] and have been used in similar modeling 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 linear in-plane torque is much larger than the out-of-plane torque (see Fig. 1).

We treat the same structure as in previous studies on Fe/MgO/Fe [19] taking into account the experimentally observed relaxation of the Fe monolayers next to the interface [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 by using a screened Korringa-Kohn-

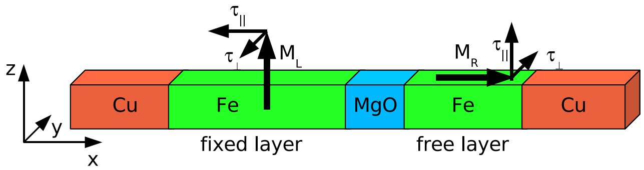

FIG. 1 (color online). Schematic geometry. The left $\vec{M}_L$ and right $\vec{M}_R$ magnetizations of the tunnel junction lie in the xz plane, at a relative angle θ (here 90°). The spin-transfer torque acts perpendicular to each magnetization and can be divided into the in-plane torque $\tau_{\|}$, which lies in the xz plane, and the out-of-plane torque $\tau_\perp$, which points in the y direction perpendicular to the plane defined by $\vec{M}_L$ and $\vec{M}_R$. For a positive voltage, the electrons flow from the fixed layer to the free layer.

Rostoker multiple scattering Green's function approach for a structure with 20 Fe monolayers in each magnetic layer. We use the frozen potential approximation to obtain potentials for junctions with different ferromagnetic layer thicknesses. In this approximation, we truncate the layers by deleting the potentials of monolayers in the interior of the layer. Below, we discuss the importance of quantum well states on transport in the Fe layers. While these quantum well states have a strong influence on the transport properties, their effect on the density and the potential is small and can be neglected.

The torque can be broken into several contributions. With no applied voltage, the in-plane torque is zero, but there can be an out-of-plane component due to interlayer exchange coupling [21]. For small voltages, we show below that for ideal junctions there are both in-plane and out-of-plane contributions, but the latter average to zero for typical thickness fluctuations. Finally, there are nonlinear contributions that are particularly important for the out-of-plane torque, in agreement with experiment.

We calculate the torque $\vec{\tau}_i$ on atomic layer i by using the change in the magnetic moment in each layer $\delta\vec{m}_i$ due to the current. The torque acting on atomic layer i is [22]

$$\vec{\tau}_i = \frac{d\vec{M}_i}{dt} = \frac{1}{\hbar}\Delta_i\hat{M}_i \times \delta\vec{m}_i, \qquad (1)$$

where $\vec{M}_i$ is the magnetic moment, $\hat{M}_i = \frac{\vec{M}_i}{M_i}$, and Δ_i is the exchange energy on atomic layer i. For a description of our implementation of the nonequilibrium Green's function technique, see Refs. [22–24]. The torkance is the variation of the torque with the voltage $d\vec{\tau}/dV$. It can be determined in linear response from the properties of the electrons at the Fermi energy

$$\frac{d\vec{\tau}_i}{dV} = \frac{1}{\hbar e}\Delta_i\hat{M}_i \times \delta\vec{m}_i(E_F), \qquad (2)$$

where $\delta\vec{m}_i(E_F) = (1/2)[\delta\vec{m}_i^L(E_F) - \delta\vec{m}_i^R(E_F)]$ contains separate contributions from electrons incident from the left and holes incident from right.

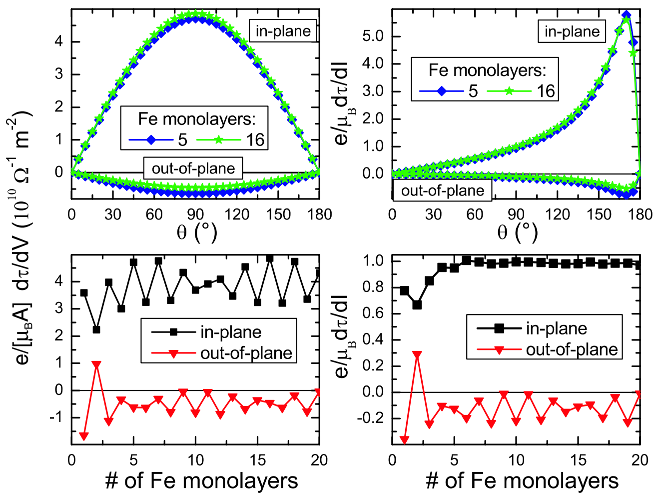

FIG. 2 (color online). Top: Torkance (left) per in-plane unit cell area A and torque per current (right) acting on the free layer as a function of the relative angle θ between the magnetizations of the Fe layers. Results are shown for different thicknesses of the free layer as indicated in the figure. Bottom: Torkance (left) and torque per current (right) as a function of the free layer thickness for an angle of 90°. All calculations have a 20 monolayer fixed layer and a 6 monolayer barrier.

Figure 2 shows *ab initio* calculations of the torkance as a function of the relative angle θ 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 torkance by the conductance $g = dI/dV$, $g(d\vec{\tau}/dI) = d\vec{\tau}/dV$. In tunnel junctions with high TMR ratios, the conductance 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 $\theta = 0°$ and 180°, respectively.

The bottom left panel in Fig. 2 shows that both the in-plane and out-of-plane torkances oscillate as a function of the Fe free layer thickness. We can fit the oscillations with a sine curve having 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 Δ_1 band in Fe at the $\bar{\Gamma}$ 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 in 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 torkance so that the oscillations in $d\tau_\perp/dI$ are even stronger than they are in the torkance. We note also that the torkance on the free layer also oscillates as a function of the fixed layer thickness (not shown).

The oscillations in the torkance arise from quantum well states in the majority channel of the Fe layers due to coherent multiple scattering. Similar oscillations in the conductance have been observed as a function of the thickness of a nonmagnetic layer inserted next to the barrier [25,26]. The effect of quantum well states on the bias dependence of the TMR has been observed in Fe/MgO/Fe/Cr [27]. Figure 3 shows quantum well states in the Fe free layer for electrons incident from the fixed layer with orientations at 90° to the free layer. The top panels show the densities of states for the majority and minority spin channels, and the bottom panels show the resulting $d\tau/dI$ for two different Fe layer thicknesses. Coherent multiple scattering causes significant differences between the majority states for the two thicknesses leading to significant differences in the out-of-plane torque and the total transmission (seen through the density in the Cu lead at the largest thicknesses in the figure). The in-plane component of the torque per current does not change.

Figure 3 also explains the restriction of the torque to the interface. The components of the nonequilibrium magnetization perpendicular to the magnetization and hence the torque arise from coherent interference between the propagating majority and evanescent minority spin components. As the minority component decays, the electrons precess around $\vec{M}_R$ within the zy plane. This precession leads to decaying oscillations of the z and y components of the conduction electrons' magnetic moments (somewhat obscured by aliasing effects). These oscillations are phase-shifted by 90° with respect to each other [28] and lead to the oscillations in the torque components having the corresponding phase shift as discussed in Fig. 2. The decay of the torque is even faster than in spin-valve systems, where the decay follows a power law due to dephasing [18].

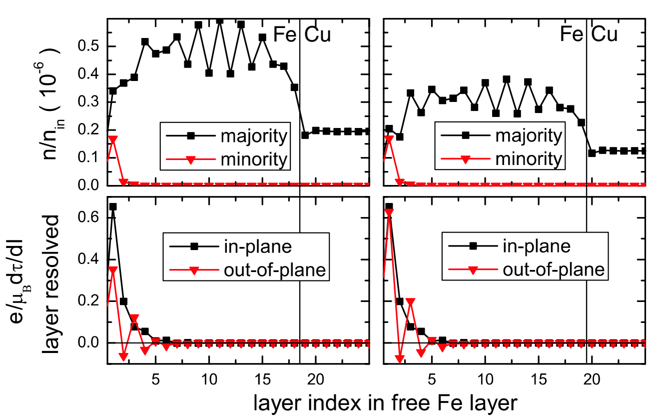

FIG. 3 (color online). Top: Layer resolved density of tunneling states n at the Fermi energy within the free Fe layer and connecting Cu layer. The density is normalized to the incident density n_{in}. Bottom: Corresponding torque components. All quantities are shown for the $\bar{\Gamma}$ point.

Note that in Fig. 2 the torque per current is very close to μ_B/e when the magnetizations are at an angle of 90°. This is expected based on a simple model of a junction between two half-metals. 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 μ_B.

Spin-transfer-driven ferromagnetic resonance quantitatively measures the magnitude and direction of the spin-transfer torque in tunnel junctions [29,30]. Tulapurkar *et al.* [29] measured a linear dependence of $\tau_\perp$ on the applied bias for small voltages (nonzero $d\tau_\perp/dV$), whereas Sankey *et al.* [31] and Kubota *et al.* [32] measured $\tau_\perp$ to be linearly independent of V but to have a significant nonlinear contribution. Sankey *et al.* compared the vanishing linear out-of-plane torque to theoretical arguments [33,34] that predict such a vanishing. However, the assumptions behind these arguments hold only for strictly symmetric junctions. We find that in ideal junctions there is a substantial out-of-plane torque even when the layers differ in thickness by a only single atomic layer. However, thickness fluctuations in a real junctions lead to cancellation of rapidly oscillating contributions as illustrated in Fig. 4. As a function of the average thickness n, the oscillations in the out-of-plane torkance cancel, and its absolute value is reduced to less than 6% of the in-plane torkance. Measuring a nonvanishing linear out-of-plane component of the torkance or oscillations of the in-plane component will require samples that are close to ideal. For most samples, the out-of-plane component will vanish.

Figure 4 shows the nonlinear bias dependence of the torque for an average free layer thickness of 19 monolayers. For absolute voltages <300 mV, the in-plane torque varies linearly with voltage, and the out-of-plane torque varies quadratically, both in agreement with experiments [31,32]

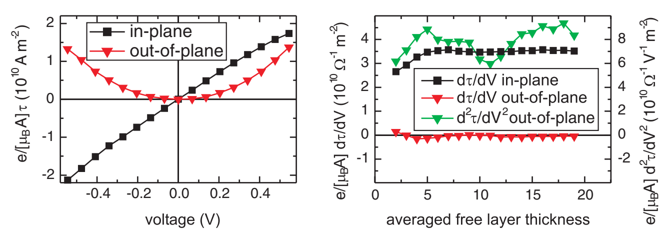

FIG. 4 (color online). Nonlinear bias dependence of the torque per in-plane unit cell area A for samples with thickness fluctuations. We assume an average free layer thickness n consisting of 50% n, 25%($n+1$), and 25%($n-1$) Fe monolayers. The fixed layer consists of equal parts 19 monolayers and 20 monolayers of Fe. The total torque is calculated by conducting the possible 6 junctions in parallel. Left: Bias dependence of the torque for an averaged free layer thickness of 19 monolayers. Right: Torkance and derivative of the torkance as a function of the averaged free layer thickness. Note that the scale is identical to the scale in the bottom left panel in Fig. 2.

and simple models [34]. The in-plane torkance measured by Sankey *et al.* [31] of $e/[\mu_B A] d\tau_{\|}/dV = 3.5 \times 10^{10} (\Omega\,\mathrm{m}^2)^{-1}$ agrees quantitatively with our calculations as does their measured quadratic out-of-plane torque coefficient of $e/[\mu_B A] d^2\tau_{\perp}/dV^2 = 6.5 \times 10^{10} (V\Omega\,\mathrm{m}^2)^{-1}$. The values reported by Kubota *et al.* [32] appear to differ by a factor of 2, which could be related to differences in the barrier thickness. This quantitative agreement between theory and experiment suggests the possibility of predictive calculations for other systems of interest. Experimentally observed deviations from the mentioned bias dependence at higher voltages can be attributed to inelastic effects that can be important at higher voltages and are not included in the present calculation.

In conclusion, spin-transfer torques in Fe/MgO/Fe tunnel junctions behave very similarly to those 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 torque comes from states around the Brillouin zone center where Fe is a half-metal with respect to the Δ_1 states. This half-metallic behavior leads to an exponential decay of the torque within the ferromagnetic layer. For a perfect sample, we calculate a small linear out-of-plane component and an oscillation of the in-plane component of the torkance as a function of the ferromagnetic layer thicknesses. Small fluctuations of the thicknesses will average out this component, in which case our calculations reproduce quantitatively the measured nonlinear bias dependence of the torque.

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