Influence of band parameters on spin-transfer torque in tunnel junctions: model calculations

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We study the in–plane spin–transfer torque in magnetic tunnel junctions for different band fillings and exchange splittings. The bias range over which the in–plane torque is linear depends strongly on these parameters. If the ferromagnetic layer is half–metallic with respect to the tunneling states, the linear bias range for the in–plane torque is significantly larger that if the behavior is metallic. For parameters that reproduce the important features of the Fe band structure, the results are in agreement with experimental data as well as with *ab initio* calculations.

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Tunnel junctions that show tunneling magnetoresistance (TMR) [1] have a variety of applications such as read heads for hard disks, magnetic sensors, and storage elements in magnetic memories. In particular, magnetic random access memories (MRAM) are of significant current interest because they have the advantages of non-volatility and lower power consumption compared to currently used random access memories are.

A typical tunnel junction which reveals the TMR effect is a magnetic multilayer structure consisting of two ferromagnets separated by an insulator. The size of the TMR effect in tunnel junctions with MgO insulating barriers exceeds several hundred percent, which is much larger than typical values of giant magnetoresistance (GMR) [2, 3]. This difference gives TMR junctions an advantage over GMR junctions for use as MRAM storage elements in magnetic random access memories . In such applications, the information is stored in the relative orientation of the two ferromagnetic layers to each other. Consequently, writing information requires that the magnetization of one of the ferromagnetic layers be easily switched while that of the other layer is typically pinned.

A promising way to switch the free layer was proposed by Slonczewski [4, 5] and Berger [6] using spin–transfer torque. This torque occurs because the tunneling electrons get polarized in one ferromagnetic layer before they tunnel through the barrier into the other ferromagnetic layer. If the magnetizations of the two ferromagnetic layers are not perfectly aligned, e.g. due to thermal fluctuations, the transport electrons will precess around the magnetization of the second layer. In turn, a torque is exerted on this magnetization which cause it to rotate. When the current is large enough the spin–transfer torque can switch the magnetization of the second layer. The dependence of the torque on the applied bias is crucial to the design of devices in which the information is written using spin–transfer torques.

The dynamics of the spin is described by the Landau–

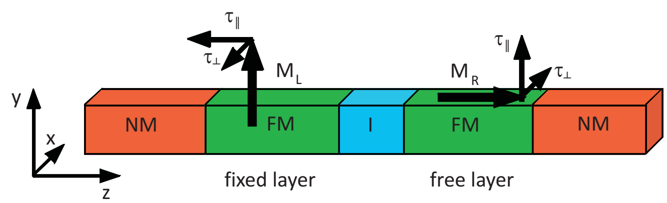

FIG. 1: Geometric structure of the magnetic tunnel junction. Two ferromagnetic (FM) layers are separated by an insulator (I). The semi-infinite leads are non–magnetic (NM). The magnetizations of the two ferromagnets are $\vec{M}_L$ and $\vec{M}_R$. The torque $\vec{\tau}$ is decomposed into the in–plane and out–of–plane component. The in–plane component lies in the plane defined by $\vec{M}_L$ and $\vec{M}_R$ and the out–of–plane torque is perpendicular to that plane.

Lifshitz–Gilbert equation [7]. The torque on the free layer $\vec{\tau}$ can be calculated by [8]

$$\vec{\tau} = \Delta \hat{M} \times \vec{m} \tag{1}$$

where Δ denotes the exchange splitting, $\hat{M} = \frac{\vec{M}}{M}$ is the direction of the magnetization $\vec{M}$ of the ferromagnetic layer, and $\vec{m}$ is the magnetization of the transport electrons.

The torque can be decomposed into two components as shown in Fig. 1 because the torque is perpendicular to the magnetization of the ferromagnetic layer. The in–plane component of the torque is in the plane spanned by the magnetizations of the two ferromagnetic layers. The out–of–plane component of the torque is perpendicular to that plane.

Experimental [9, 10] as well as theoretical investigations [11–14] show a quadratic bias dependence for the out–of–plane component of the torque. However, the results differ for the in–plane torque. Sankey *et al.* [9] measured a linear dependence of the in–plane torque for applied biases up to 400 mV, which agrees quantitatively with *ab initio* calculations by Heiliger and Stiles [11]. On

TABLE I: Tight-binding band parameters t (hopping) and E_{bo} (bottom of the band) for the different regions. For the ferromagnet and the insulator parameters were taken from Ref. [16]. In particular, these parameters are a representation of real Fe and MgO Δ_1 bands. The bottom of the band of the majority spin and the exchange splitting Δ are varied in our calculations

region	$t_\uparrow = t_\downarrow$ (eV)	$E_{bo\uparrow}$ (eV)	$E_{bo\downarrow}$ (eV)
ferromagnet (FM)	2.5	variable	$E_{bo\uparrow} + \Delta$
insulator (I)	0.64	2.8	2.8
non-magnet (NM)	5.0	-10.0	-10.0

the other hand, experimental results by Kubota *et al.* [10] show strong non–linear dependence of the in–plane torque on applied bias voltages larger than 100 mV, as found in the model calculations by Theodonis *et al.* [13] and Xiao *et al.* [12].

This controversy has been partially resolved through experimental and theoretical progress. Recent experimental investigations by Wang *et al.* [15] argue that the bias dependence in Fe/MgO/Fe should be linear as found in the ab initio calculations [11]. Further Kalitsov *et al.* [14] showed using a simple band model that the band filling and the exchange field can drastically change the bias dependence of the in–plane torque. However, the band widths they use are much smaller than for those real Fe bands, so they only find linear behavior after integrating over parallel wave vectors. In this paper we show that even a one–dimensional one–band model gives a linear voltage dependence for the in–plane torque using band parameters consistent with realistic Fe bands.

For our investigation we use a one–band model. The multilayer is divided into five regions sketched in Fig. 1. The thickness of the insulator is three times the bulk lattice constant, those of the ferromagnets are five times the bulk lattice constant, and the non-magnetic layers are semi-infinite. In the case of Fe/MgO/Fe tunnel junctions this corresponds to six monolayers of MgO and 10 monolayers of Fe. We use incoming and outgoing plane waves for the wave functions in each region, but the values of the wave vectors are chosen from a tight-binding band structure. The parameters of the band structure for the different regions are given in Table I. They are chosen according to the Δ_1 bands in the real system. We restrict the calculation to the Δ_1 bands because [3] the Δ_1 states dominate the transport in MgO based tunnel junctions.

We look at different band fillings in the ferromagnetic layers by changing the bottom of the band in these layers. In addition, we change the exchange splitting between 1 eV and 4 eV. For Δ =2 eV and E_{bottom} =-1 eV we have a Δ_1 band close to the real Δ_1 band in Fe. Changes of the exchange splitting and band filling can be achieved experimentally e.g. by alloying or using different magnetic materials.

Without an applied bias the in–plane component of the torque is zero because the in–plane component is not invariant under time inversion. Consequently, if a bias voltage is applied, computing the in-plane torque only requires integrating over an energy window between the electro–chemical potentials of both leads. The out–of–plane component of the torque is invariant under time inversion so that there is a finite contribution even in the absence of a bias voltage. This zero-bias out–of–plane component is the interlayer exchange coupling. Calculating the out–of–plane component is much more demanding than calculating the in-plane component because it requires integration over energy over all occupied states.

In the present calculation we do not attempt to compute the out–of–plane torque. Since the tight-binding model is chosen to the accurate close to the Fermi energy, there is no reason to believe that the other occupied states are a reasonable description of the Fe bands. In particular, it is very hard to get agreement with experimental data for both components with the same set of parameters. Although one–band models produce [12] the quadratic dependence of the out–of plane torque, the size has not been correctly reproduced. For these reasons, we restrict ourselves in the following to the in–plane component of the torque where the one–band model provides an adequate description.

The applied bias voltage is modelled by shifting the band structure of the layers left (right) from the barrier by half of the voltage up (down). Fig. 2 shows the in–plane torque as a function of the applied bias for three chosen parameter sets of our investigation. There is a strong dependence on the exchange splitting. For large exchange splittings the range of linear behavior for the in–plane component of the torque extend up to at least 300 mV depending on the band filling. For an exchange splitting of 2 eV as in Fe (middle panel in Fig. 2) the behavior of the curves depends strongly on the band filling. In the case of E_{bo} =-1 eV which represents real Fe the bias dependence is linear up to 300 mV. This result is in agreement with experimental data [9] and *ab initio* results [11] for MgO based tunnel junctions. With increasing band filling the range of linear behavior in the bias dependence is substantially reduced. With further decreased exchange splitting the range of linear behavior is quite small (left panel in Fig. 2). In this case the bias dependence of the in–plane component of the torque is in agreement with other model calculations [12, 13]. In particular, for small voltages there can be a linear behavior which becomes non–linear for larger voltages.

To understand the different mechanisms that lead to the different bias dependencies one has to analyze the band structure. In general, there are two possible scenarios. The ferromagnetic layer can be half-metallic with respect to the tunneling states or it can be metallic. In other words, only one spin band is present at the Fermi

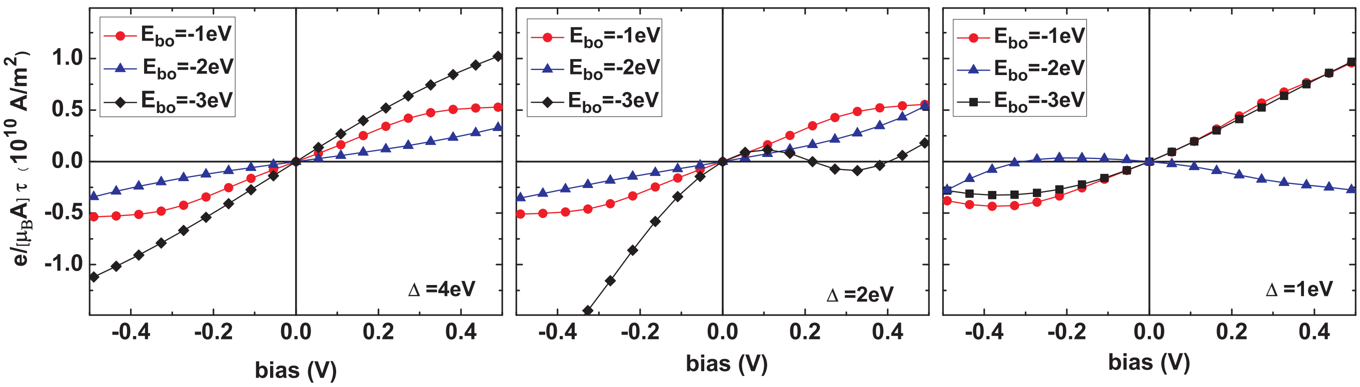

FIG. 2: The in–plane component of the torque as a function of the applied bias for three different values of the exchange field Δ. For each exchange field we plot the curves for three different band fillings that are controlled by the bottom of the band E_{bo}.

TABLE II: The character of the ferromagnetic layers and the bias dependence for different band parameters. Depending on the band parameters the ferromagnetic layer can be metallic (M) or half-metallic (HM). The bias dependence is mainly linear (L) or non-linear (NL). For the analysis of the bias dependence we restrict ourselves to a bias voltage between -300 mV and 300 mV.

	Δ =4 eV	Δ =2 eV	Δ =1 eV
E_{bo} =-1 eV	HM / L	HM / L	M / NL
E_{bo} =-2 eV	HM / L	M / NL	M / NL
E_{bo} =-3 eV	HM / L	M / NL	M / NL

level or both are. This leads to a qualitative difference in the precession of electrons injected into the ferromagnetic layer. In the half-metallic case, the precession decays exponentially because the electron state is a superposition of a propagating majority state and an evanescent minority state. In the metallic case, both spin states are propagating, leading to a precession which does not decay. In the latter case there is a strong influence of the thickness of the ferromagnetic layer on the spin-transfer torque. In the half-metallic case there can also be a small change of the linear slope of the in–plane component of the torque due to quantum well states within the ferromagnetic layer [11].

It is easy to determine if the ferromagnet is metallic or half-metallic at a certain bias voltage determined by analyzing the band parameters. In Table II we characterize the band structure and the bias dependence of the in–plane torque. For the latter we look at the bias range between -300 mV and 300 mV. From this table we see a clear connection between the linear (non-linear) bias dependence and the half-metallic (metallic) character of the ferromagnet.

In conclusion, our calculations of the in-plane torque show that the different results of experiments and calculations can be understood by varying the band filling and the exchange field. By changing these parameters, e.g. by alloying or using different magnetic materials, various bias dependencies of the in-plane torque can be obtained. The different bias dependencies originate in the metallic and half-metallic character of the ferromagnetic layers for different energies depending on the band parameters.

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[1] J. Moodera, L. Kinder, T. Wong, and R. Meservey, Phys. Rev. Lett. bf 74, 3273 (1995).
[2] G. Binasch, P. Grünberg, F. Saurenbach, and W. Zinn, Phys. Rev. B bf 39, 4828 (1989).
[3] C. Heiliger, P. Zahn, and I. Mertig, Mater. Today bf 9, 4 (2006).
[4] J. Slonczewski, Phys. Rev. B bf 39, 6995 (1989).
[5] J. Slonczewski, J. Magn. Magn. Mater. bf 159, L1 (1996).
[6] L. Berger, Phys. Rev. B bf 54, 9353 (1996).
[7] T. L. Gilbert, IEEE Transactions on Magnetics bf 40, 6 (2004).
[8] C. Heiliger, M. Czerner, B. Yu. Yavorsky, I. Mertig, M. D. Stiles, J. Appl. Phys. bf 103, 07A709 (2008).
[9] J. C. Sankey, Y.–T. Cui, J. Z. Sun, J. C. Slonczewski, R. A. Buhrman, and D. C. Ralph, Nature Phys. bf 4, 67 (2008).
[10] H. Kubota, A. Fukushima, K. Yakushiji, T. Nagahama, S. Yuasa, K. Ando, H. Maehara, Y. Nagamine, K. Tsunekawa, D. D. Djayaprawira, N. Watanabe, and Y. Suzuki, Nature Phys. bf 4, 37 (2008).
[11] C. Heiliger and M. D. Stiles, Phys. Rev. Lett. bf 100, 186805 (2008).
[12] J. Xiao, G. E. W. Bauer, A. Brataas, Phys. Rev. B bf 77, 224419 (2008).
[13] I. Theodonis, N. Kioussis, A. Kalitsov, M. Chshiev, and W. H. Butler, Phys. Rev. Lett. bf 97, 237205 (2006).
[14] A. Kalitsov, M. Chshiev, I. Theodonis, N. Kioussis, W. H. Butler, Phys. Rev. B bf 79, 174416 (2009).
[15] C. Wang, Y.-T. Cui, J. Z. Sun, J. A. Katine, R. A. Buhrman, D. C. Ralph, Phys. Rev. B bf 79, 224416 (2009).

[16] T. Z. Raza and H. Raza, arXiv:0804.2557v5 (2009).