Thin Solid Films 519 (2011) 8247–8251

Contents lists available at ScienceDirect

Thin Solid Films

journal homepage: www.elsevier.com/locate/tsf

Spin transfer torque and tunneling magnetoresistance dependences on finite bias voltages and insulator barrier energy

Chun-Yeol You [a,*], Jae-Ho Han [b], Hyun-Woo Lee [b]

[a] Department of Physics, Inha University, Incheon 402-751, Republic of Korea
[b] PCTP and Department of Physics, POSTECH, Pohang 790-784, Republic of Korea

ARTICLE INFO

Available online 1 April 2011

Keywords:
Spin transfer torque
Tunneling magnetoresistance
Insulator barrier
Finite bias voltage

ABSTRACT

We investigate the dependence of perpendicular and parallel spin transfer torque (STT) and tunneling magnetoresistance (TMR) on the insulator barrier energy of the magnetic tunnel junction (MTJ). We employed the single orbit tight binding model combined with the Keldysh non-equilibrium Green's function method in order to calculate the perpendicular and parallel STT and the TMR in the MTJ with finite bias voltages. The dependences of the STT and TMR on the insulator barrier energy are calculated for semi-infinite half metallic ferromagnetic electrodes. We find a perfect linear relation between the parallel STT and the tunneling current for a wide range of insulator barrier energy. Furthermore, the TMR also depends on the insulator barrier energy, contradicting Julliere's simple model.

1. Introduction

The spin transfer torque (STT) [1,2] and tunneling magnetoresistance (TMR) are key technologies in current magnetism research due to their potential application in STT-MRAM (magnetoresistive random access memory) [3]. The information writing mechanism of STT-MRAM is so-called current induced magnetization switching (CIMS) based on STT phenomena in a magnetic tunneling junction (MTJ). Since the STT occurs by angular momentum transfer by spin polarized electron current, the system is far from equilibrium. Therefore, a rigorous non-equilibrium treatment such as Keldysh non-equilibrium Green's function methods must be employed [4–6]. Well established Keldysh non-equilibrium Green's function methods have been successfully adopted to explain recent experimental observations for STT in MgO based MTJs [7–9]. The STT has two components, parallel (in-plane) and perpendicular (out-of-plane). In our coordinate system, the parallel (perpendicular) STT is denoted as T_x (T_y), respectively. It is well known that the perpendicular STT is small in all metallic systems [10].

In metallic systems, the whole Fermi surface contributes to Brillouin zone integration, and the perpendicular STT rapidly decays. However, it is quite different in the MTJ system, where an insulator layer exists between two electrodes. It has been theoretically predicted and experimentally confirmed that the perpendicular STT is comparable to the parallel STT in the MTJ [6–8]. The difference between a metallic system and a MTJ originates from the in-plane momentum, $k_{||}$, integral in the Brillouin zone [10]. The insulator barrier acts as a $k_{||}$ filter, and hence $k_{||}$s around the Γ point mainly contribute to integration in the MTJ system. Furthermore, the perpendicular STT is important in practical spin dynamics. Since the perpendicular STT is an even function of the bias voltage in a symmetric MTJ [11], either parallel or anti-parallel states are preferred for both signs of the bias voltages, and the effect increases for higher bias. Therefore, it is important to understand the details of the spin dynamics. The spin dynamics(?) may cause back-hopping, which is switching back after once current induced magnetization switching has occurred [12].

In this study, we calculate the dependences of the STT and TMR on the insulator barrier energy height in the frame of the Keldysh non-equilibrium Green's function method with finite bias voltage [4–6,13]. A free electron, single orbit, tight binding model is used in our calculations for simple cubic half metallic semi-infinite ferromagnetic electrodes. We find that the perpendicular (out-of-plane) STT is an even function of the bias voltage, and lower barrier energy gives a larger STT. Since the perpendicular STT is the same as interlayer exchange coupling, roughly speaking, the magnitude exponentially decreases with the barrier height. The parallel (in-plane) STT is neither an even nor odd function of the bias voltage. The parallel STT also decreases with the barrier height, but the dependence is not a simple exponential. However, we find a perfect linear relation between the parallel STT and the total tunneling current. The TMR shows strong bias dependence, although we did not consider inelastic scattering. The strong bias dependences are mainly due to the band shift [14,15]. At the finite bias, the TMR depends on the barrier height, which contradicts to Julliere's simple model [16].

* Corresponding author.
E-mail address: cyyou@inha.ac.kr (C.-Y. You).

0040-6090/$ – see front matter
doi:10.1016/j.tsf.2011.03.057

2. Keldysh non-equilibrium Green's function method

We briefly summarize the Keldysh non-equilibrium Green's function method for the STT calculations in our study. More details can be found elsewhere [5,10]. A schematic sketch of the trilayer structure is shown in Fig. 1(a). The left and right electrodes are semi-infinite, and a finite $N(=5)$ insulator barrier layer is placed between them. We assumed that the left (right) electrode is a polarizer (switching) layer. The magnetization direction of the polarizer layer is placed in the xz-plane with angle θ from the positive z-axis. The magnetization direction of the switching layer is parallel to the positive z-axis. From semi-infinite electrodes, we calculate the surface Green's function and then each insulator layer is added by the Dyson equation [17–19]. We considered a single-orbit tight-binding model with a simple cubic structure, and two ferromagnetic electrodes are considered to be identical. The exchange energy, $\Delta_{\rm EX}$, of the ferromagnetic layer is 0.7 eV, and the on-site energy of spin up (down) is 2.3 eV (3.0 eV). For simplicity, half metal ferromagnetic electrodes are examined, and the hopping energy, $t_{hop}=-0.5$ eV, is fixed for all layers. The on-site energy of the insulator barrier layer, $U_{\rm Ins}$, is varied from 3.5 to 4.5 eV. Corresponding barrier energy heights, $V_{\rm Ins}(=U_{\rm Ins}-6|t_{hop}|)$, are 0.5–1.5 eV. The on-site energy inside of the insulator barrier decreases linearly as $U_{Ins}(i)=U_{Ins}-i\ V_{Bias}/N$ with the bias voltage V_{Bias}, and i is the index number. With finite bias voltage, the spin current at $(n-1)$-th layer is defined by [5,6]

$$\langle \mathbf{j}_{n-1}\rangle = \frac{1}{2}\sum_{k_{\parallel}}\int\frac{d\omega}{2\pi}\mathrm{Tr}\left\{\left[G^{+}_{RL}(\omega)T-G^{+}_{LR}(\omega)T^{\dagger}\right]\boldsymbol{\sigma}\right\}. \quad (1)$$

More details and the meanings of each symbol are described in Ref. [5]. The charge current is easily obtained by replacing $\boldsymbol{\sigma}/2$ with the unit matrix multiplied by $e/\hbar$. The spin current is directly related with STT by $\mathbf{T}=\langle \mathbf{j}_{Ins}\rangle$ at the interface between the insulator and switching layer for the semi-infinite switching layer. Therefore, we can obtain the parallel and perpendicular STT with the charge current. In our study, the pessimistic definition of $\mathrm{TMR}=(R_{AP}-R_P)/R_{AP}$ is used; therefore, the TMR of half metal is 100% with small bias voltage, which corresponds to the infinite TMR in the optimistic definition.

3. Spin transfer torque and tunneling magnetoresistance for various insulator energies

According to Slonczewski [16,20], the STT is related with the magneto-conductance coefficients, and the *torkance* is given by

$$\frac{d\dot{\mathbf{S}}_R}{dV} = \frac{\hbar}{4e}(G_{++}-G_{--}+G_{+-}-G_{-+})\mathbf{s}_R\times(\mathbf{s}_R\times\mathbf{s}_L). \quad (2)$$

Hence, they strongly depend on the insulator barrier energy height. Therefore, it is easy to imagine that the STT also strongly depends on the insulator barrier energy. The insulator barrier energy of MgO is a fixed value for a bulk, but this does not hold for a thin film in a real MTJ stack. The barrier energy can be tailored by the deposition and annealing conditions [21,22]. The low resistance-area product (RA) is another important parameter for real device applications, due to impedance matching in STT-MRAM, as well as a better data read rate and noise consideration in the hard disk read head [23]. The RA mainly depends on the insulator barrier thickness

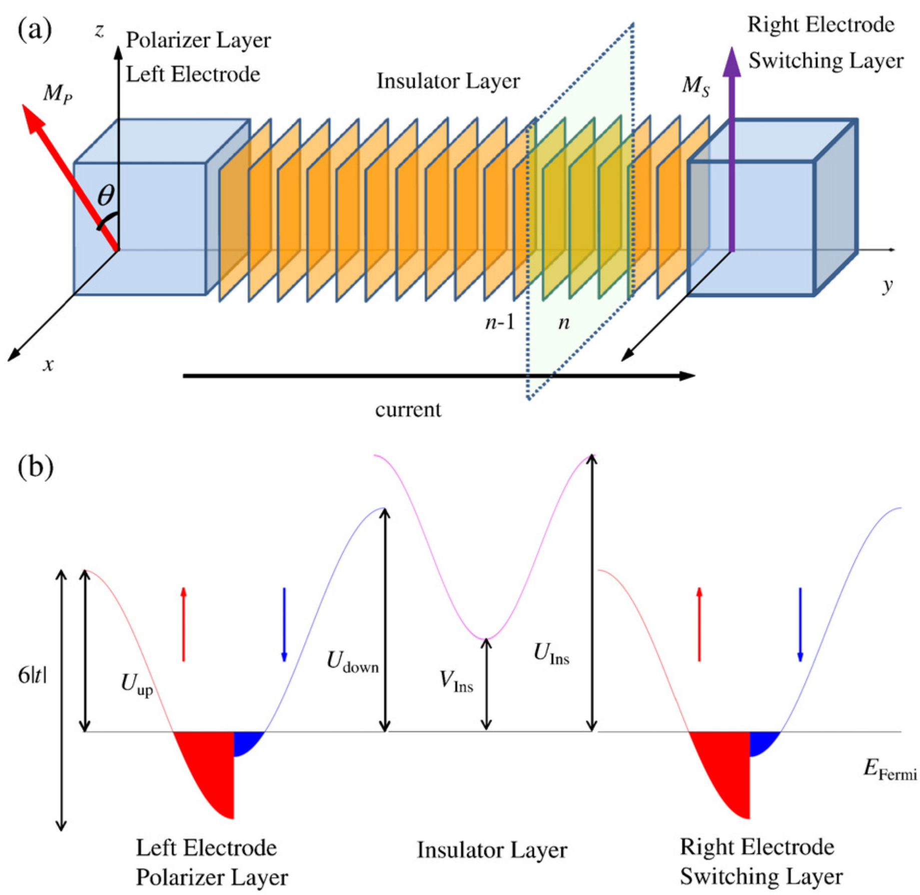

Fig. 1. (a) Schematic diagram of the MTJ layer structure. The semi-infinite left and right ferromagnetic leads are connected with the insulator layer. The direction of the magnetization of the polarizer layer is placed in the xz-plane with an angle θ from the positive z-axis. The magnetization direction of the switching layer is parallel to the positive z-axis. (b) Band structures of the ferromagnetic and insulator layers.

and the energy height. These parameters can be optimized by careful fabrication conditions. Therefore, the study of the STT and TMR dependences on the barrier energy height is an important research subject.

3.1. Tunneling magnetoresistance

Before discussing STT, let us discuss the tunneling current and TMR. We depicted the tunneling current as a function of the barrier energy height, V_{Ins}, for $V_{Bias}=0.1$ and 1.0 V in Fig. 2. The tunneling current is calculated for $\theta=0$, $\pi/2$, and π, respectively. In these calculations, we find the following: While a simple WKB approximation gives exponential dependence of the tunneling current on $\sqrt{V_{Ins}}$ [24], our results show slight deviation from simple exponential dependence. We plotted the log–log scale for comparison with the WKB approximation. Furthermore, the slope of the decay also depends on the bias voltage and θ. For $V_{Bias}=0.1$ V case, the anti-parallel state ($\theta=\pi$) shows smaller tunneling current, that is, larger resistance than the parallel state ($\theta=0$). However, the converse results are obtained for the large bias ($V_{Bias}=1.0$ V), implying a negative TMR (as shown in Fig. 4). The V_{Ins} dependent TMR is shown in Fig. 3 for $V_{Bias}=0.1$ and 1.0 V. The TMR is determined by the spin polarized density of state in the framework of Julliere's model [25], and it implies that the TMR is independent of the barrier energy height. However, our Keldysh non-equilibrium Green's function results show barrier energy height dependence. For small V_{Bias} (=0.1 V), the dependence is weak. However, it is more serious for large V_{Bias} (=1.0 V), as shown in Fig. 3. Even the sign of the TMR is changed for larger V_{Bias} in our results. It must be pointed out that the TMR is measured with the finite bias voltage in real device operation. The bias dependences of the TMR are also plotted in Fig. 4 for selected V_{Ins} (=0.5–1.5 eV). It is widely accepted that the decrease of the TMR with bias voltage is mainly due to the magnon excitation. However, the magnon excitation is not considered in our calculation. Therefore, the decrease of the TMR is ascribed to the band shifts with the bias voltage [14,15]. At zero bias, we obtain 100% TMR (pessimistic) due to the half-metallic nature of the ferromagnetic layers. As we already noted, the present results show much more complex behavior than Julliere's simple model. Julliere's model fails to describe the huge TMR in a MgO based MTJ. The huge TMR in a MgO based MTJ can be explained by the in-plane momentum conservation due to the epitaxial structure with band symmetry selected tunneling [26–29]. Even though we do not consider the band symmetry selected tunneling in order to mimic a MgO based TMR, we can conclude

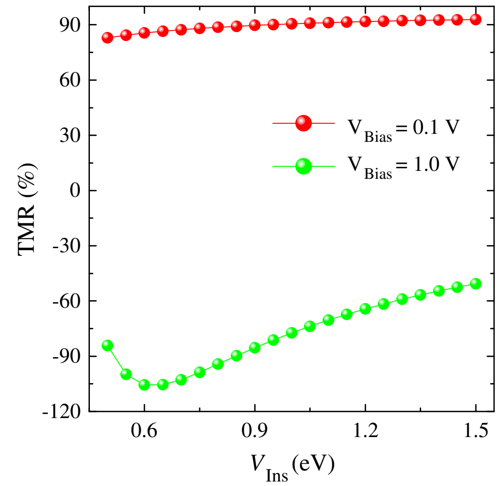

Fig. 3. TMR (pessimistic) as a function of V_{Ins} for $V_{Bias}=0.1$ and 1.0 V.

that Julliere's model is too simple to describe the correct TMR with finite bias voltage, and the barrier energy height must be considered in TMR study.

3.2. Perpendicular and parallel STT

Next, the perpendicular and parallel STT are considered. Since the STT is closely related with the spin dependent conductance, it must be sensitive to the barrier energy height. The dependences of perpendicular (T_y) and parallel (T_x) STT on the V_{Ins} are depicted in Fig. 5(a) and (b) for $V_{Bias}=0.1$ and 1.0 V, respectively. All STT results are calculated for $\theta=\pi/2$. The overall behavior of the perpendicular STT is exponential decay with V_{Ins}. In particular, $V_{Bias}=0.1$ V appears to show perfect exponential decay. However, more careful analysis reveals that there is a small deviation. A somewhat large deviation is found in the small V_{Ins} region for $V_{Bias}=1.0$ V case. In this region, the perpendicular STT is negative and we omitted negative values in order to make a log-scale plot. The exponential dependences can be easily explained by the relation between the STT and spin dependent conductance. Notably, since the perpendicular STT is related with the interlayer exchange coupling, the exponential dependence is natural [30]. However, the origin of the slight deviation from the exponential dependence is not clear. We also performed the same calculations with non-half-metal ferromagnetic layers, and stronger deviations

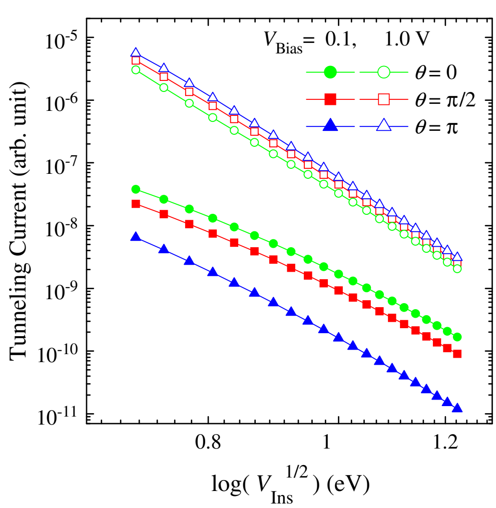

Fig. 2. Tunneling current ($\theta=0$, $\pi/2$, π) as a function of $\sqrt{V_{Ins}}$ for $V_{Bias}=0.1$ and 1.0 V. For comparison with the WKB approximation, we used log–log plot.

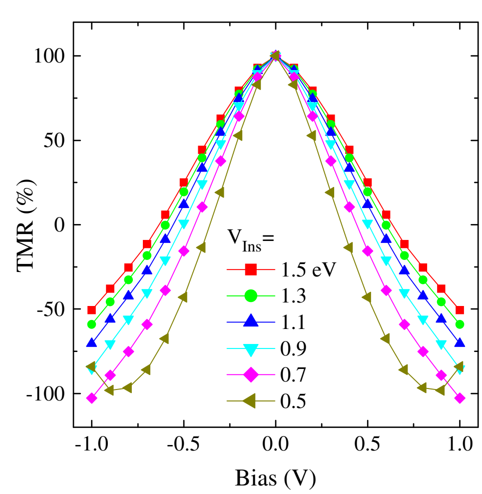

Fig. 4. Bias dependent TMR (pessimistic) as a function of $V_{Bias}=0.1$ and 1.0 V for various V_{Ins}(=0.5–1.5 eV).

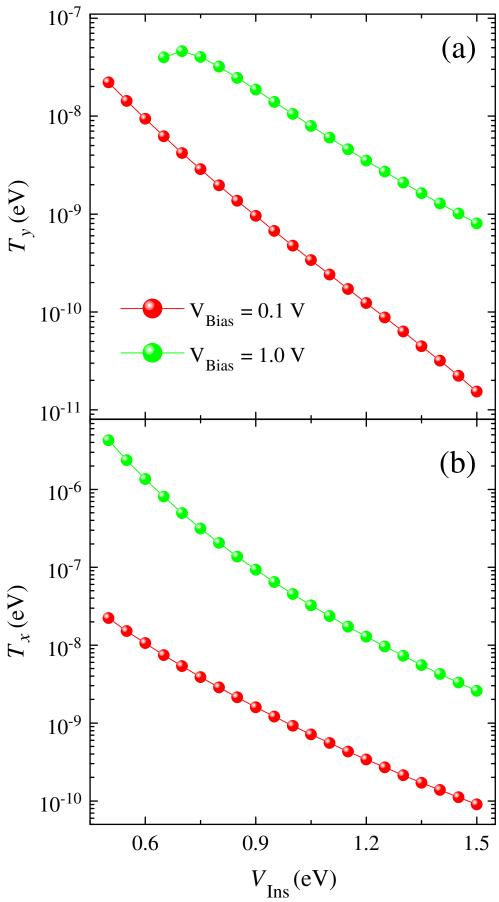

Fig. 5. (a) Perpendicular (T_y) and (b) parallel (T_x) STT as a function of V_{Ins} for $V_{Bias}=0.1$ and 1.0 V.

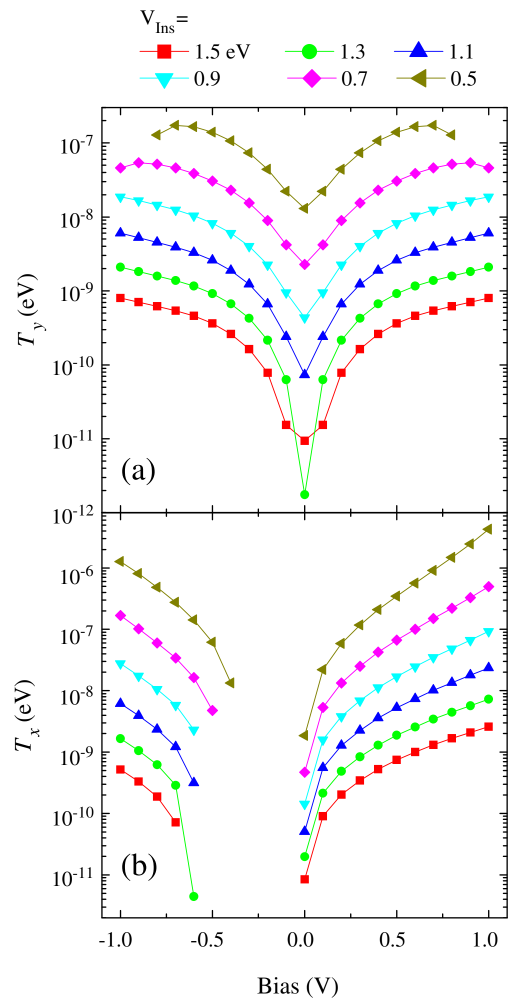

Fig. 6. (a) Perpendicular (T_y) and (b) parallel (T_x) STT as a function of V_{Ins} for $V_{Bias}=0.1$ and 1.0 V. (The negative values are omitted for the log-scale plots.)

from the exponential dependence were found (not shown here). It must be pointed out that the magnitude of the STT is very sensitive to the barrier energy height: a lower barrier gives a larger STT for a given bias voltage. Therefore, lower barrier energy height guarantees more effective current induced magnetization switching.

The bias dependences of the perpendicular and parallel STT for selected V_{Ins}(=0.5–1.5 eV) are shown in Fig. 6(a) and (b). Here, we also omitted the negative STT for log-scale plots. The perpendicular STT is an even function of V_{Bias} for all V_{Ins} by the symmetry. However, the parallel STT is neither an even nor odd function, as Theodonis explained [6].

Fig. 7 shows the perpendicular and parallel STT as a function of the current for a given $V_{Bias}=0.1$ and 1.0 V. The current values for each V_{Ins} ($\theta=\pi/2$) in Fig. 2 are used as abscissa data with the corresponding perpendicular and parallel STT. We find perfect linearity between the parallel STT (T_x) and the total charge current. Surprisingly, all data points of T_x for $V_{Bias}=0.1$ and 1.0 V fall onto a single linear curve in spite of the wide range of current values. However, the perpendicular STT (T_y) shows a large deviation from the linear relations. The perfect linear relation of T_x is delineated by Eq. (2), while the perpendicular STT has a more complicated relation. In the parallel STT case, only the states between the left and right electrode Fermi energies contribute, as is also the case for the tunneling current. However, all occupied states from the bottom of the energy band to the Fermi energy contribute to the perpendicular STT.

It must be emphasized that the parallel STT is directly related with the tunneling current, which deviates slightly from the perfect exponential dependence on V_{Ins} in Fig. 2. Therefore, the total current and parallel STT are not perfect exponential functions of V_{Ins}, but they have a linear relation with each other. This may provide a clue to the following question: Which is a more fundamental driving force of the STT, the current or the voltage in the MTJ?

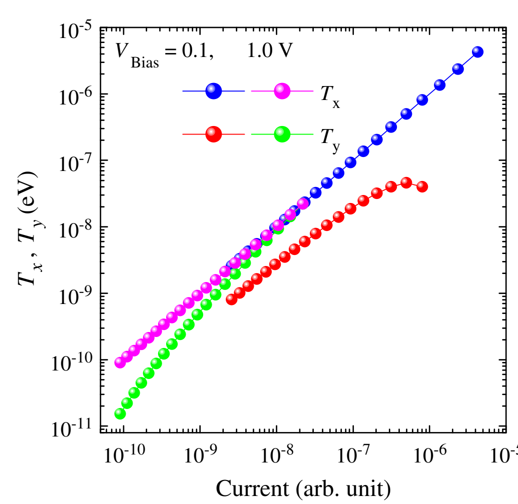

Fig. 7. Perpendicular (T_y) and parallel (T_x) STT as a function of total current. The current values from Fig. 2 ($\theta=\pi/2$) for various V_{Ins} with fixed V_{Bias}, and the corresponding STT values are plotted.

4. Conclusion

We investigate the TMR and STT in the frame of the non-equilibrium Green's function method for a symmetric MTJ. We varied the insulator barrier energy height. We found that the TMR shows more complicated bias voltage and barrier height dependences than Julliere's simple model. Furthermore, the perpendicular and parallel STT show approximately exponential decay with the barrier energy height with somewhat unexpected deviations. However, we found a perfect linear relation between the parallel STT and the total tunneling current, which implies a relation between the parallel STT and tunneling current. Here, it must be noted that our reported results are not unique features of the half-metallic ferromagnetic electrode. We also found similar trends for the non-half-metallic ferromagnetic electrode, although the results are not presented here for simplicity.

Acknowledgements

This work was supported by the Nano R&D (2008-02553) and Mid-career Researcher Program (2010-0014109) programs through a NRF grant funded by MEST.

References

[1] J.C. Slonczewski, J. Magn. Magn. Mater. 159 (1996) L1.
[2] L. Berger, J. Appl. Phys. 49 (1978) 2156;
L. Berger, Phys. Rev. B 54 (1996) 9353.
[3] R. Beach, et al., Tech. Digest IEDM (2008) 08-305;
T. Kishi, et al., Tech. Digest IEDM (2008) 08-309.
[4] L.V. Keldysh, JETP 20 (1965) 1018.
[5] D.M. Edwards, F. Federici, J. Mathon, A. Umerski, Phys. Rev. B 71 (2005) 054407.
[6] I. Theodonis, N. Kioussis, A. Kalitsov, M. Chshiev, W.H. Butler, Phys. Rev. Lett. 97 (2006) 237205.
[7] H. Kubota, A. Fukushima, K. Yakushiji, T. Nagahama, S. Yuasa, K. Ando, H. Maehara, Y. Nagamine, K. Tsunekawa, D.D. Kjayaprawira, N. Watanabe, Y. Suzuki, Nat. Phys. 4 (2008) 37.
[8] J.C. Sankey, Y.-T. Cui, J.Z. Sun, J.C. Slonczewski, R.A. Buhrman, D.C. Ralph, Nat. Phys. 4 (2008) 67.
[9] S.-C. Oh, S.-Y. Park, A. Manchon, M. Chshiev, J.-H. Han, H.-W. Lee, J.-E. Lee, K.-T. Nam, Y. Jo, Y.-C. Kong, B. Dieny, K.-J. Lee, Nat. Phys. 5 (2009) 898.
[10] P.M. Haney, C. Heiliger, M.D. Stiles, Phys. Rev. B 79 (2009) 054405.
[11] J.C. Slonczewski, Phys. Rev. B 71 (2005) 024411.
[12] T. Min, J.Z. Sun, R. Beach, D. Tang, P. Wang, J. Appl. Phys. 105 (2009) 07D126.
[13] Chun-Yeol You, J. Magnetics 12 (2007) 72.
[14] S.O. Valenzuela, D.J. Monsma, C.M. Marcus, V. Narayanamurti, M. Tinkham, Phys. Rev. Lett. 94 (2005) 196601.
[15] B.G. Park, T. Banerjee, J.C. Lodder, R. Jansen, Phys. Rev. Lett. 99 (2007) 217206.
[16] M. Julliere, Phys. Lett. A 54 (1975) 225.
[17] J. Mathon, Phys. Rev. B 56 (1997) 11810.
[18] J. Mathon, A. Umerski, Murielle Villeret, Phys. Rev. B 55 (1997) 14378.
[19] J. Mathon, Murielle Villeret, A. Umerski, R.B. Muniz, J. d'Albuquerque e Castro, D.M. Edwards, Phys. Rev. B 56 (1997) 11797.
[20] J.C. Slonczweski, J.Z. Sun, J. Magn. Magn. Mater. 310 (2007) 169.
[21] R.C. Sousa, J.J. Sun, V. Soares, P.P. Freitas, A. Kling, M.F. da Silva, J.C. Soares, Appl. Phys. Lett. 73 (1998) 3288.
[22] Y. Nagamine, H. Maehara, K. Tsunekawa, D.D. Djayaprawira, N. Watanabe, S. Yuasa, K. Ando, Appl. Phys. Lett. 89 (2006) 162507.
[23] K. Tsunekawa, et al., Appl. Phys. Lett. 87 (2005) 072503.
[24] J.J. Sakurai, Modern Quantum Mechanics, Addison-Wesley, 1993.
[25] M. Julliere, Phys. Lett. A 54 (1975) 225.
[26] W.H. Butler, X.-G. Zhang, T.C. Schulthess, J.M. MacLaren, Phys. Rev. B 63 (2001) 054416.
[27] J. Mathon, A. Umerski, Phys. Rev. B 63 (2001) 220403(R).
[28] S. Yuasa, T. Nagahama, A. Fukushima, Y. Suzuki, K. Ando, Nat. Mater. 3 (2004) 868.
[29] S.S.P. Parkin, C. Kaiser, A. Panchula, P.M. Rice, B. Hughes, M. Samant, S.-H. Yang, Nat. Mater. 3 (2004) 862.
[30] P. Bruno, Phys. Rev. B 52 (1995) 411.