

October 2006

# Self-consistent simulation of quantum transport and magnetization dynamics in spin-torque based devices

Sayeef Salahuddin

*Purdue University - Main Campus, [ssalahud@purdue.edu](mailto:ssalahud@purdue.edu)*

Supriyo Datta

*Network for Computational Nanotechnology, Birck Nanotechnology Center, and Purdue University, [datta@purdue.edu](mailto:datta@purdue.edu)*

Follow this and additional works at: <http://docs.lib.purdue.edu/nanopub>

---

Salahuddin, Sayeef and Datta, Supriyo, "Self-consistent simulation of quantum transport and magnetization dynamics in spin-torque based devices" (2006). *Birck and NCN Publications*. Paper 191.

<http://docs.lib.purdue.edu/nanopub/191>

This document has been made available through Purdue e-Pubs, a service of the Purdue University Libraries. Please contact [epubs@purdue.edu](mailto:epubs@purdue.edu) for additional information.

# Self-consistent simulation of quantum transport and magnetization dynamics in spin-torque based devices

Sayeef Salahuddin<sup>a)</sup> and Supriyo Datta

School of Electrical and Computer Engineering, Purdue University, West Lafayette, Indiana 47907 and NSF Network for Computational Nanotechnology (NCN), Purdue University, West Lafayette, Indiana 47907

(Received 21 June 2006; accepted 24 August 2006; published online 11 October 2006)

This letter presents a self-consistent solution of quantum transport, using the nonequilibrium Green's function method, and magnetization dynamics, using the Landau-Lifshitz-Gilbert formulation. This model is applied to study "spin-torque" induced magnetic switching in a device where the transport is ballistic and the free magnetic layer is sandwiched between two antiparallel (AP) ferromagnetic contacts. A hysteretic current-voltage characteristic is predicted at room temperature, with a sharp transition between the bistable states that can be used as a nonvolatile memory. It is further shown that this AP pentalayer device may allow significant reduction in the switching current, thus facilitating integration of nanomagnets with electronic devices. © 2006 American Institute of Physics. [DOI: 10.1063/1.2359292]

Successful integration of nanomagnets with electronic devices may enable the first generation of practical spintronic devices, which have been elusive so far due to stringent requirements such as low temperature and high magnetic field. It was predicted by Slonczewski<sup>1</sup> and Berger<sup>2</sup> that magnetization of a nanomagnet may be flipped by a spin polarized current through the so-called "spin-torque" effect and this was later demonstrated experimentally.<sup>3,4</sup> However, the early spin-torque systems were metal based that allowed only a small change in the magnetoresistance. In addition, metallic channels are difficult to integrate with complementary metal oxides semiconductor technology. Recently a number of experiments have demonstrated current induced magnetization switching in MgO based tunneling magnetoresistance (TMR) devices at (i) room temperature (ii) with a TMR ratio of more than 100% and (iii) without any external magnetic field.<sup>5,6</sup> Encouraged by these experimental results, here we explore theoretically a memory device based on current induced magnetization switching in the quantum transport regime.

The device under consideration is shown in Fig. 1. It consists of five layers. The two outer layers are "hard magnets" which act as spin polarized contacts. There is a soft magnetic layer inside the channel whose magnetization is affected by the current flow through the so-called spin-torque effect. The channel can be a semiconductor<sup>7</sup> or a tunneling oxide.<sup>6</sup> Note that the contacts are arranged in an antiparallel (AP) configuration. We have recently showed that in this configuration, the torque exerted by the injected electrons on a the nearby spin array (in this case the soft magnet) is maximum.<sup>8</sup> A similar prediction was also made by Berger<sup>9</sup> based on expansion/contraction of the Fermi surface. The possibility of an enhanced torque and therefore a lower switching current is our motivation for the pentalayer configuration instead of the conventional trilayer geometry.

In Fig. 1, the soft magnet changes the transport through its interaction with the channel electrons, which in turn exert a torque on the magnet and try to rotate it from its equilibrium state. In this letter, we present a self-consistent solution

of both these processes: the transport of channel electrons [through nonequilibrium Green's function (NEGF)] and the magnetization dynamics of the free layer [through Landau-Lifshitz-Gilbert (LLG) equations] [see Fig. 1(b)]. Our calculations show clear hysteretic  $I$ - $V$  suggesting possible use as a memory. Furthermore, we show that a pentalayer device with AP contact as shown in Fig. 1(a) should exhibit a significant reduction in the switching current.

Unlike the conventional metallic spin-torque systems, where transport is predominantly diffusive, the transport in semiconductors or tunneling oxides is ballistic or quasiballistic. This necessitates a quantum description of the transport. We use the NEGF method to treat the transport rigorously. The interaction between channel electrons and the ferromagnet is mediated through exchange and it is described by  $H_I(\mathbf{r}) = \sum_{R_j} J(\mathbf{r} - \mathbf{R}_j) \boldsymbol{\sigma} \cdot \mathbf{S}_j$ , where  $r$  and  $R_j$  are the spatial coordinates and  $\boldsymbol{\sigma}$  and  $S_j$  are the spin operators for the channel electron and  $j$ th spin in the soft magnet.  $J(\bar{r} - \bar{R}_j)$  is the interaction constant between the channel electron and the  $j$ th spin in the magnet. This interaction is taken into account through self-energy ( $\Sigma_s$ ), which is a function of the magnetization ( $\mathbf{m}$ ), using the so-called self-consistent Born approximation.<sup>10</sup> In this method, the spin current flowing into the soft magnet is given by

$$[I_{\text{spin}}] = \int dE \frac{e}{\hbar} i [\text{Tr} \{ G \Sigma_s^{\text{in}} - \Sigma_s^{\text{in}} G^\dagger - \Sigma_s G^n + G^n \Sigma_s^\dagger \}], \quad (1)$$

where the trace is taken only over the space coordinates. Then  $[I_{\text{spin}}]$  is a  $2 \times 2$  matrix in the spin space. Here,  $G$  denotes Green's function. The torque exerted on the magnet is calculated from  $[I_{\text{spin}}]$  by writing  $T_i = \text{Trace} \{ S_i [I_{\text{spin}}] \}$ , where  $i = \{x, y, z\}$ . The total current, which is found from a similar expression as Eq. (1) with the self-energy  $\Sigma_s$  now replaced by the total self-energy  $\Sigma$ ,<sup>11</sup> is shown in Figs. 2(a) and 2(b) for two different configurations of the magnetization. The nonlinearity in the  $I$ - $V$  follows from the spin-flip exchange interaction<sup>8</sup> which is usually ignored in a purely barrier model.

For the calculations, the Hamiltonian was written in the effective-mass approximation where the hopping parameter

<sup>a)</sup>Electronic mail: ssalahud@purdue.edu

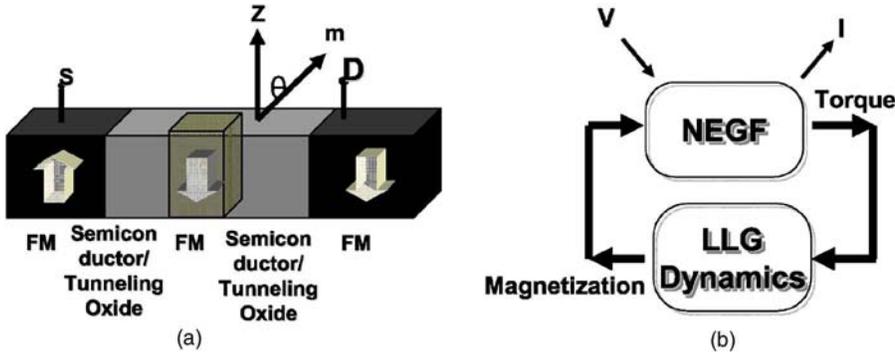


FIG. 1. (Color online) (a) Schematic showing the pentalayer device. The free ferromagnetic layer is embedded inside the channel which is sandwiched between two “hard” ferromagnetic contacts. (b) A schematic showing the self-consistent nature of the transport problem. The magnetization dynamics and transport are mutually dependent on one another.

$t = \hbar^2 / (2m^* a^2)$ ,  $m^* = 0.7m_e$  (Ref. 12) denoting the effective mass and  $a$  being the lattice spacing. The interaction constant  $J$  is assumed to be 0.01 eV.<sup>13</sup> A sample set of parameters is  $E_f = 2$  eV, barrier height = 1.2 eV;<sup>12</sup> barrier width = 1 nm, and exchange splitting = 1.2 eV.<sup>14</sup> However, the barrier height, width, and exchange splitting were artificially varied to get desired injection efficiency and TMR value. We also modified the perfect-contact self-energy to read  $\Sigma = -t' \exp(ika)$  ( $t' \neq t$  and  $k$  is the momentum) to simulate the reflective nature of the contact (for details see Ref. 15). For plots 2–4, an injection efficiency of 70% was assumed.

The magnetization dynamics is simulated using the LLG equation

$$(1 + \alpha^2) \frac{\partial \mathbf{m}}{\partial t} = \gamma (\mathbf{m} \times \mathbf{H}_{\text{eff}}) - \frac{\gamma \alpha}{m} \mathbf{m} \times \mathbf{m} \times \mathbf{H}_{\text{eff}} + \text{current torque.} \quad (2)$$

Here,  $\mathbf{m}$  is the magnetization of the soft magnet,  $\gamma = 17.6$  MHz/Oe is the gyromagnetic ratio, and  $\alpha$  is the Gilbert damping parameter. The  $\mathbf{H}_{\text{eff}} = \mathbf{H}_{\text{ext}} + (2Ku_2/M_s)m_z \hat{z} - (2Ku_p/M_s)m_x \hat{x}$ , where  $H_{\text{ext}}$  is the externally applied magnetic field,  $M_s$  is the saturation magnetization, and  $Ku_2$  and  $Ku_p$  are the uniaxial and in-plane anisotropy constants, respectively. The conventional LLG equation has to be solved with the current torque ( $T_i$ ) that works as an additional source term.

Figure 2 shows the situations when the transport and magnetization dynamics are independent of each other. This will change when Eqs. (1) and (2) are solved self-consistently. If we start from  $\theta = \pi$  position,  $I$ - $V$  curve follows the trend shown in Fig. 2(a). However, once the torque exceeds the critical field (discussed later), the magnet switches abruptly. As a result  $I$ - $V$  characteristics now follow that shown in Fig. 2(b). This results in the hysteretic  $I$ - $V$  shown in Fig. 3(a).

Figure 3(b) shows current flow in the device in response to read-write-read pulse sequence. Here, we have used read pulse of 0.5 V and write pulse of +1 V. The soft magnet is initially in the  $\theta = \pi$  position. The write pulse switches it to  $\theta = 0$ . Note the change in the current level in response to the read pulse before and after applying the write pulse.

A question may be raised regarding the asymmetric  $I$ - $V$  of Fig. 2, which is not expected if one thinks about the device in Fig. 1(a) as a series combination of two devices, one antiparallel (AP) and one parallel (P). The device, however, is different from a mere series combination since the contact in the middle works as a mixing element for up and down spin electrons. The difference will be clear if one assumes 100% injection efficiency. No current is expected to flow

through the series combination of an AP and a P device. However, in our device, a current can still flow because the contact in the middle mixes the up and down spin channels. This “extra” current originating from “channel mixing” gives the observed asymmetry in Fig. 2.

Since electronic time constants are typically in the subpicosecond regime which is much faster than the magnetization dynamics (typically of the order of nanoseconds), we have assumed that, for electronic transport, the magnetization dynamics is a quasistatic process.<sup>16</sup>

The switching is obtained by the torque component which is transverse to the magnetization of the soft magnet. From Eq. (2), considering average rate of change of energy, it can be shown that the magnitude of the torque required to induce switching is  $\alpha \gamma (H_{\text{ext}} + H_k + H_p/2)$ ,<sup>17</sup> where  $H_k = 2Ku_2/M_s$  and  $H_p = 2Ku_p/M_s = 4\pi M_s$ . This then translates into a critical spin current magnitude of

$$I_{\text{spin}} = \frac{2e}{\hbar} \alpha (M_s V) (H_{\text{ext}} + H_k + 2\pi M_s). \quad (3)$$

Here,  $V$  is the volume of the free magnetic layer. Depending on the magnitudes of  $\alpha$ ,  $M_s$ ,  $H_k$ , and thickness  $d$  of the magnet, the spin current density to achieve switching varies from  $10^5$  to  $10^6$  A/cm<sup>2</sup> (e.g., for Co, using typical values  $\alpha \sim 0.01$ ,  $H_k \sim 100$  Oe,  $M_s = 1.5 \times 10^3$  emu/cm<sup>3</sup>, and  $d = 2$  nm, the spin current density required is roughly  $10^6$  A/cm<sup>2</sup>). Note that this requirement on spin current is completely determined by the magnetic properties of the free layer. The actual current density is typically another factor of 10–100 larger due to the additional coherent component of the current which does not require any spin flip. Hence an important metric for critical current requirement is  $r = I_{\text{coherent}}/I_{\text{spin}}$ , which should be as small as possible. Intuitively, with AP

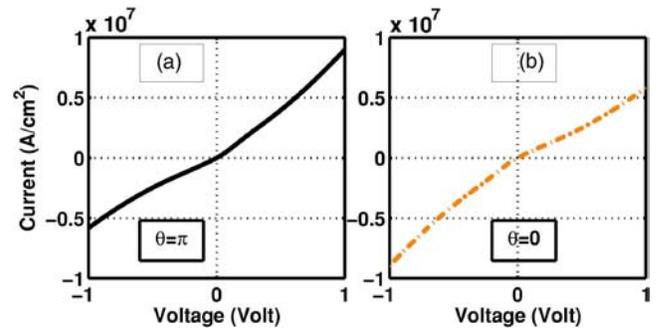


FIG. 2. (Color online) Nonself-consistent (with magnetization dynamics)  $I$ - $V$  characteristics of the proposed device (a) with the soft magnet initially at  $\theta = \pi$  position. The current is larger for positive bias (b) with the soft magnet initially at  $\theta = 0$  position. The current is larger for negative bias.

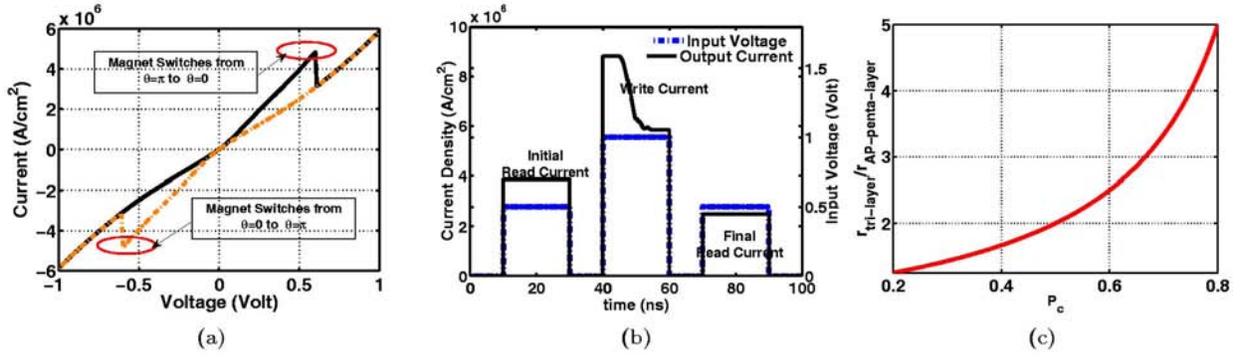


FIG. 3. (Color online) (a) The hysteretic  $I$ - $V$  originating from a self-consistent solution of transport and LLG. At a certain bias, the current torque produced by the conduction electrons is strong enough to flip the magnet. These transition points are indicated in the figure. (b) Response to a Read-Write-Read pulse. The write pulse switches the magnet from  $\theta=\pi$  to  $\theta=0$ . The corresponding change in the current can be clearly seen during the write pulse. (c) Variation of the ratio of  $r_{\text{trilayer}}/r_{\text{AP-pentala-layer}}$  ( $r=I_{\text{coherent}}/I_{\text{spin}}$ ), showing the possible reduction of switching current for the AP pentalayer device compared to the 3-layer device.

contacts, the coherent current  $I_{\text{coherent}} \propto t^2 \alpha \beta$ , where  $t$  is the hopping matrix element,  $\alpha$  is the majority(minority) density of states for the injecting contact, and  $\beta$  is the minority(majority) density of states of the drain contact. Similarly the spin-flip current  $I_{\text{sf}} \propto J^2 [\alpha^2 (1 - P_\alpha) - \beta^2 P_\alpha]$ , where  $P_\alpha$  is the probability of a spin in the free layer to be in state  $\alpha$ .<sup>8</sup> It follows that

$$r_{\text{AP}} = \frac{I_{\text{coherent}}}{I_{\text{sf}}} \Big|_{\text{AP}} = \frac{t^2}{J^2} \frac{1 - P_c^2}{P_c + [(1/2) - P_\alpha](1 + P_c^2)}, \quad (4)$$

where  $P_c = (\alpha - \beta) / (\alpha + \beta)$  indicates the degree of contact polarization. This approximate analytical expression [Eq. (4)] agrees quite well with detailed NEGF calculations described above. The  $I_{\text{coherent}}$  and  $I_{\text{spin}}$  can be found, respectively, from the symmetric and asymmetric portions of the nonlinear  $I$ - $V$  shown in Fig. 2. Figure 3(c) shows the variation of  $g = r_{\text{trilayer}}/r_{\text{AP-pentala-layer}}$  with  $P_c$ . The plot shows that  $g \gg 1$  for reasonable values of  $P_c$ , indicating a lower switching current for the pentalayer device. Recent experiments on AP pentalayer devices<sup>18–20</sup> have shown similar reduction of switching current compared to tri-layer devices. These experiments seem to follow the general trends of Fig. 3(c) as the reduction factor is seen to increase with increasing TMR (see Fig. 4 of Ref. 19). A detailed study of the dependence of the reduction factor on material parameters is beyond the scope of this letter.

The sharp transition between high and low states in Fig. 3(a) arises from the bistable nature of the solutions to the LLG equation in the absence of any external field perpendicular to the easy axis. The intrinsic speed depends on  $\omega = \gamma B$  where  $B$  can be roughly estimated as  $B \sim \hbar T / (2\mu_B)$ . A higher speed will require higher current density.

In conclusion, we have shown a scheme for calculating the “spin current” and the corresponding torque directly from transport parameters within the framework of NEGF formalism. A nonlinear  $I$ - $V$  is predicted for AP pentalayer devices. Experimental observation of this nonlinearity [which can also be detected as steps or peaks in, respectively, the first and second derivative of the  $I$ - $V$  (Ref. 8)] would provide strong confirmation of our approach. We have further

coupled the transport formalism with the phenomenological magnetization dynamics (LLG equation). Our self-consistent simulation of NEGF-LLG equations show clear hysteretic switching behavior, which is a direct consequence of the nonlinearity described above. Finally, we have shown that the switching current for AP pentalayer devices can be significantly lower than that of the conventional trilayer devices.

This work was supported by the MARCO Focus Center for Materials, Structure and Devices.

- <sup>1</sup>J. C. Slonczewski, J. Magn. Mater. **159**, L1 (1996).
- <sup>2</sup>L. Berger, Phys. Rev. B **54**, 9353 (1996).
- <sup>3</sup>S. I. Kiselev, J. C. Sankey, I. N. Krivorotov, N. C. Emley, R. J. Schoelkopf, R. A. Buhrman, and D. C. Ralph, Nature (London) **425**, 380 (2003).
- <sup>4</sup>J. A. Katine, F. J. Albert, R. A. Buhrman, E. B. Myers, and D. C. Ralph, Phys. Rev. Lett. **84**, 3149 (2000).
- <sup>5</sup>H. Kubota, A. Fukushima, Y. Ootani, S. Yuasa, K. Ando, H. Maehara, K. Tsunekawa, D. D. Djayaprawira, N. Watanabe, and Y. Suzuki, Jpn. J. Appl. Phys., Part 2 **44**, L1237 (2005).
- <sup>6</sup>S. S. P. Parkin, C. Kaiser, A. Panchula, P. M. Rice, B. Hughes, M. Samant, and S. H. Yang, Nat. Mater. **3**, 862 (2004).
- <sup>7</sup>X. Jiang, R. Wang, R. M. Shelby, R. M. Macfarlane, S. R. Bank, J. S. Harris, and S. S. P. Parkin, Phys. Rev. Lett. **94**, 056601 (2005).
- <sup>8</sup>S. Salahuddin and S. Datta, Phys. Rev. B **73**, 081301R (2006).
- <sup>9</sup>L. Berger, J. Appl. Phys. **93**, 7693 (2003).
- <sup>10</sup>S. Datta, Proceedings of the International School of Physics Enrico Fermi, Italiana di Fisica, 2005, p. 1.
- <sup>11</sup>S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, Cambridge, 1995).
- <sup>12</sup>W. H. Rippard, A. C. Perrella, F. J. Albert, and R. A. Buhrman, Phys. Rev. Lett. **88**, 046805 (2002).
- <sup>13</sup>A. H. Mitchell, Phys. Rev. **105**, 1439 (1957).
- <sup>14</sup>F. J. Himpsel, Phys. Rev. Lett. **67**, 2363 (1991).
- <sup>15</sup>S. Datta, *Quantum Transport: Atom to Transistor* (Cambridge University Press, Cambridge, 2005).
- <sup>16</sup>S. Salahuddin and S. Datta, <http://www.arxiv.org/cond-mat/0606648>.
- <sup>17</sup>J. Z. Sun, Phys. Rev. B **62**, 570 (2000).
- <sup>18</sup>G. D. Fuchs, I. N. Krivorotov, P. M. Braganca, N. C. Emley, A. G. F. Garcia, D. C. Ralph, and R. A. Buhrman, Appl. Phys. Lett. **86**, 152509 (2005).
- <sup>19</sup>Y. M. Huai, M. Pakala, Z. T. Diao, and Y. F. Ding, Appl. Phys. Lett. **87**, 222510 (2005).
- <sup>20</sup>H. Meng, J. Wang, and J.-P. Wang, Appl. Phys. Lett. **88**, 082504 (2006).

Applied Physics Letters is copyrighted by the American Institute of Physics (AIP). Redistribution of journal material is subject to the AIP online journal license and/or AIP copyright. For more information, see <http://ojps.aip.org/aplo/aplcr.jsp>