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

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

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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 and Berger 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. 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. 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 or a tunneling oxide. Note that the contacts are arranged in an antiparallel (AP) configuration. We have recently shown that in this configuration, the torque exerted by the injected electrons on the nearby spin array (in this case the soft magnet) is maximum. A similar prediction was also made by Berger 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

\[ H_{I}(r) = \sum_{ij} J_{ij}(r) \sigma_{i} \cdot \sigma_{j}, \]

where \( r \) and \( r_{j} \) are the spatial coordinates and \( \sigma_{i} \) and \( \sigma_{j} \) are the spin operators for the channel electron and the \( j \)th spin in the soft magnet. \( J(r-r_{j}) \) 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 \( \Sigma_{i} \), which is a function of the magnetization \( \langle m \rangle \), using the so-called self-consistent Born approximation. In this method, the spin current flowing into the soft magnet is given by

\[ [I_{\text{spin}}] = \int d\mathbf{r} \frac{e}{\hbar} [\text{Tr}(G^{\text{in}} \Sigma_{i} G^{\text{out}} - \Sigma_{i} G^{\text{out}} G^{\text{in}})] \]
magnetization dynamics are independent of each other. This width, and exchange splitting were artificially varied to get consistently. If we start from $K_{\text{up}}/H_{20849}$ and assume that, for electronic transport, the magnetization dynamics is a quasistatic process.16

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.10

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 $\alpha \gamma (H_{\text{ext}} + H_k + H_p)/2$,17 where $H_k = 2K_{\text{up}}/M_s$ and $H_p = 2K_{\text{up}}/M_s = 4\pi M_s$. This then translates into a critical spin current magnitude of

$$I_{\text{spin}} = \frac{2e}{h} \alpha (M_s V) (H_{\text{ext}} + H_k + 2\pi M_s).$$ (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 $10^9$ to $10^6$ A/cm$^2$ (e.g., for Co, using typical values $\alpha \sim 0.01$, $H_k \sim 100$ Oe, $M_s = 1.5 \times 10^5$ emu/cm$^3$, and $d = 2$ nm, the spin current density required is roughly $10^6$ A/cm$^2$). 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 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.

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.
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 of the injecting contact, and $\beta$ is the minority(majority) density of states of the drain contact. Similarly the spin-flip current $I_{sf} \propto \beta^2 \alpha^2 (1 - P_a - \beta^2 P_a)$, where $P_a$ is the probability of a spin in the free layer to be in state $\alpha$. It follows that

$$r_{AP} = \frac{I_{\text{coherent}}}{I_{sf}} = \frac{t^2}{J^2} \frac{1 - P_c^2}{P_c + [(1/2) - P_a] (1 + P_c^2)},$$

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 $g = r_{\text{triangle}} / r_{\text{AP pentalayer}}$ with $P_c$. The plot shows that $g \approx 1$ for reasonable values of $P_c$, indicating a lower switching current for the pentalayer device. Recent experiments on AP pentalayer devices $^{18-20}$ 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 $B \approx hT/(2\mu_B)$. 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.

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