Self-consistent Quantum Transport and Magnetization Dynamics in STT-RAM

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A self-consistent simulation model for STT-RAM (Spin-Torque Transfer magnetic-RAM) is presented which uses the Non Equilibrium Green's Function (NEGF) method to solve quantum transport equations for the exerted torque in the free layer, coupled with macrospin dynamics solved using the Landau-Lifshitz-Gilbert equation in the presence of the torque. The simulations are done self-consistently, to account for the continual change in interspin angle and torque during the evolution of the free spin. Simulations are done with a parameterized model using a continuum effective mass model for a quick evaluation of the resulting I-Vs and R-Vs, assuming abrupt interfaces. Switching in a half metallic like Fe contacts in Fe/MgO/Fe magnetic tunnel junction (MTJ) is studied.

***Index Terms*—Modeling, Quantum Theory, Torque, Tunneling**

I. INTRODUCTION

Tunneling based spin torque transfer (STT) devices have recently stimulated a lot of attention due to their room temperature operation, reasonably good Tunneling Magnetoresistance (TMR), low power writing capacity and overall scalability. Slonczewski[1] and Berger [2] independently predicted in 1996 that the magnetization of a nanomagnet may be flipped by a spin polarized current through the so-called "spin-torque" effect. The advancement of MgO-based Magnetic Tunnel Junction (MTJ) with high TMR (> 100%) has further revolutionized the STT-RAM industry [3]. High TMR values require high polarization factors and spin transfer efficiency leading to greatly decreased switching currents in MgO MTJs. Crystalline Fe/Mg)/Fe[100] MTJ has been of great interest in the field of Spintronics for its high tunneling magnetoresistance value that originates from up spin Δ_1 symmetry at the center of the Brillouin zone(Γ point)[4]. The TMR has been shown to exceed 1000% theoretically [5]-[6] and the highest value achieved at room temperature is 180% [7]. In this paper, we study spin torque transfer switching in a Fe/MgO/Fe MTJ.

The device under consideration is shown in Fig 1. The magnetization of left Fe ferromagnetic layer, M_p, is pinned towards +z axis by exchange coupling with antiferromagnetic layer, and is known as the pinned layer. The magnetization of the right layer, M, with the x-z as the easy-plane, can change freely with any applied field, and is therefore known as the free layer. A self-consistent STT-RAM model is used to study the system that calculates the transport and exerted torque of channel electrons through Non-Equilibrium Green's function (NEGF) and the magnetization dynamics of the free layer through Landau-Lifshitz-Gilbert (LLG) equations. Calculations are done using a parameterized NEGF model assuming abrupt ferromagnet-barrier interfaces.

II. MICRO MAGNETIC SIMULATION

The torque exerted on the free-layer is calculated by the current divergence at the ferromagnet-barrier interface, as spin transfer torque is nothing but a measure of how much angular momentum was transferred from the current to the magnet. By invoking the conservation of angular momentum, one can then calculate the total momentum transfer or torque, by looking at the net momentum flow into the free ferromagnet [8].

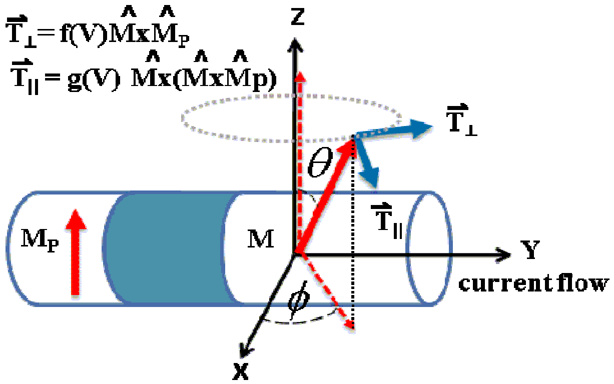

Fig. 1. Schematic of a STT-RAM with parallel anisotropy. M_P is the magnetization of the left pinned Ferromagnet (FM) contact which is fixed along the +Z axis. The right free FM contact has a magnetization of M with the Z as the easy axis and X-Z as the easy-plane. $T_\perp$ is the torque exerted perpendicular to the plane and is given by $f(V)MxM_P$ where V is the voltage applied. $T_{||}$ is the torque exerted parallel to the plane and is given by $g(V)MxMxM_P$.

$$\vec{T} = -\mu_{\mathrm{b}} \int dV * \vec{\nabla}.\vec{J} \qquad (1)$$

where μ_b is the Bohr Magneton, V is the volume of the free ferromagnet, and $\vec{\nabla}.\vec{J}$ is the current divergence. The torque $\vec{T}$ is composed of $\vec{T}_{\perp}(\|)$, exerted parallel to the easy-plane and $\vec{T}_\perp$ exerted perpendicular to the easy-plane. Both $\vec{T}_{\perp}(\|)$ and $\vec{T}_\perp$ are dependent on voltage [9]. The individual torque components parts are fed into a single-domain Landau-Lifshitz-Gilbet (LLG) equation is given by,

$$\frac{d\widehat{M}}{dt} = \mu_0 \gamma \widehat{M} \times \overrightarrow{Heff} + \alpha \widehat{M} \times \frac{d\widehat{M}}{dt} + \frac{\vec{T}_\perp}{Vol * M_S} + \vec{T}\Big\|\frac{\square}{Vol*M}\Big]_S$$

(2)

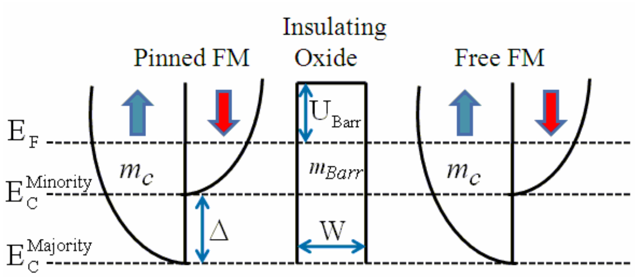

Fig. 2. Band structure of magnetic tunnel junction (MTJ). FM contacts are described by splitted bands for up and down spins, while the oxide introduces a barrier. E_F $E_C^{Majority}$ and $E_C^{Minority}$ are the Fermi level, bottom of majority spin conduction band, and bottom of minority spin conduction band respectively. W is the width of the insulating barrier. m_C and m_{Barr} are the effective masses in the contact and barrier respectively.

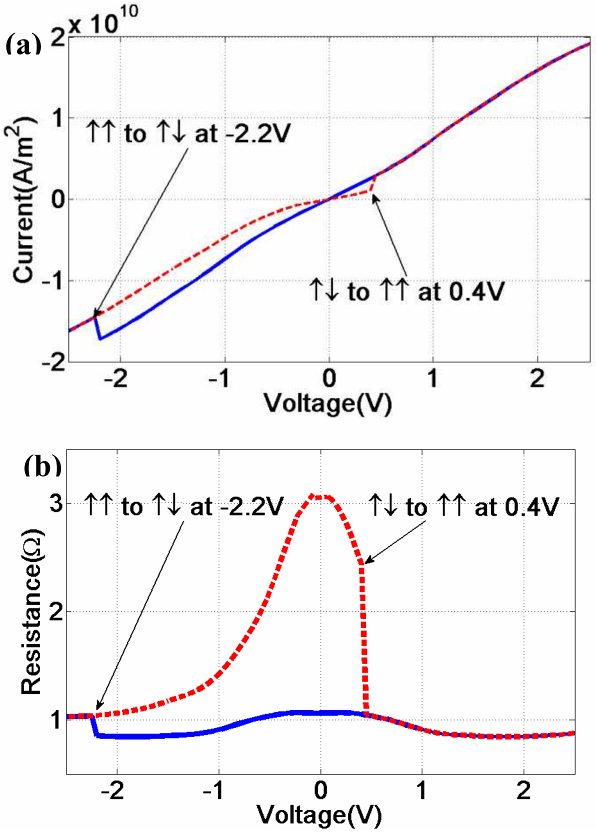

Fig.3 (a) Current-voltage and (b) Resistance-voltage originating from a self-consistent solution of parameterized NEGF and LLG models for an elliptical Fe/MgO(0.84 nm)/Fe STT-RAM (major axis=40µm, minor axis=30µm)At -2.2V, the MTJ state switches from . parallel to anti-parallel state and anti-parallel to parallel at 0.4V

where $\widehat{M}$ is the unit vector of the free layer, γ is the gyromagnetic ratio, μ_0 is vacuum permeability, α is the damping parameter , M_S is the saturation magnetization and Vol is volume of the free layer. $\overrightarrow{Heff}$ is the effective field due to magnetocrystalline anisotropy and easy-plane anisotropy [10] and α is the damping constant. The LLG equation is solved numerically by the method specified in [10]. The critical current is then given by [10]-11]:

$$I_C = \frac{2e}{\eta\hbar} M_S V \alpha (H_K + 2\pi M_s) \qquad (3)$$

where H_K is the anisotropy field and η, the polarization at the contacts. For the free Fe ferromagnet, α is taken to be 0.01, M_S is $1710 \times \frac{10^3 A}{m}$, and anisotropy constant K is $4.8 \times \frac{10^4 J^3}{m}$ [12]. Therefore, the critical switching current is around ~10^{10}A/m^2 which is really high.

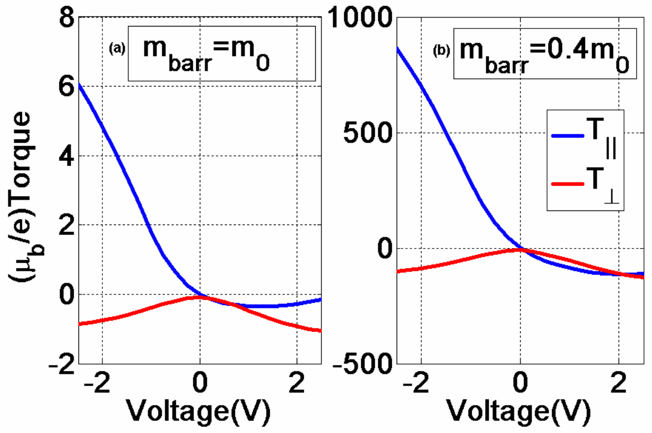

Fig. 4. Effect of barrier mass on switching. When compared to effective barrier mass of m_0 in fig. (a) ,decreased effective barrier mass produces more $T_{\parallel}$ which accounts for the faster switching in the Fe/MgO/Fe MTJ. The effective barrier mass in our Fe/MgO/Fe MTJ is 0.4 m_0.

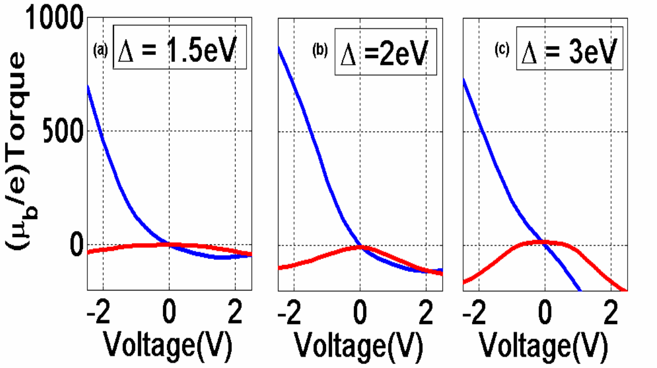

Fig. 5. (a) Effect of band splitting on torque. (a) Δ=1.5eV or 40% polarization, (b)Δ=2eV (Fe/MgO/Fe) or 92% polarization and (c) Δ=3eV or 100% polarization. Increased polarization results in increased out-of-plane torque that hampers parallel to anti-parallel switching.

III. Fe/MgO/Fe Parameterized Single-Band Model

The theoretical formulation is based on the Non-Equilibrium Green's Function (NEGF) method discussed extensively at [14]. Fig 2 shows the band diagram of the Fe/MgO/Fe MTJ , where U_{Barr} is the barrier offset between the contact and the insulator, E_F is Fermi-level , Δ is the band splitting between majority and minority spin electrons, and W is the width of the insulator. m_C and m_{Barr} are the effective masses in the contact and barrier respectively. The above specified parameters were fitted to the experimental results of Fe/MgO/Fe tunneling in [7]. U_{Barr} is taken to be 3.5eV, E_F at 2.25eV , Δ of 2.0eV that results in 92% current polarization, and a barrier width of 0.8nm to ensure high enough current for the ferromagnet to switch. m_C and m_{Barr} are taken to be 0.4 m_0 and 1.2m_0 respectively where m_0 is the mass of free electron.

IV. Fe/MgO/Fe STT-RAM SIMULATION RESULTS

Fig. 3 shows current-voltage and resistance-voltage originating from a self-consistent solution of parameterized NEGF and LLG models for an elliptical Fe/MgO(0.84 nm)/Fe STT-RAM (major axis=40μm, minor axis=30μm)At -2.2V, the MTJ state switches from parallel to anti-parallel state and anti-parallel to parallel at 0.4V. A pulse width of 25ns was used. It can be seen in the fig. 3 the parallel to anti-parallel switching and anti-parallel to parallel switching is highly asymmetric. The asymmetry ratio is 69%.

The asymmetry of the switching is due to the high polarization of the nearly half metallic nature of the Fe contacts. In our simulation, the torque for positive voltage corresponds to switching from anti-parallel to parallel states or from high resistance to low resistance, and the torque for negative voltage corresponds to switching in the reverse order. The negetive magnitude of the out-of-plane torque in the simulation aids magnetization switching from the antiparallel to the parallel state and inhibits magnetization switching from the parallel to the antiparallel state. In Fig. 4, we can see the effect of effective barrier mass on the in-plane torque. When compared to effective barrier mass of m_0 in fig. (a) ,decreased effective barrier mass produces more $T_\parallel$ which accounts for the faster anti-parallel to parallel switching in the Fe/MgO/Fe MTJ. The effective barrier mass in our Fe/MgO/Fe MTJ is 0.4 m_0. Fig. 4 shows the effect of band splitting on torque. (a) Δ=1.5eV or 40% polarization, (b) Δ=2eV (Fe/MgO/Fe) or 92% polarization and (c) Δ=3eV or 100% polarization. Increased polarization results in increased out-of-plane torque that hampers parallel to anti-parallel switching. Therefore, the 92% spin polarization in the nearly half metallic iron contacts results in higher negative voltage parallel to anti-parallel switching. In half-metals (100% polarization), there is no switching at all.

V. CONCLUSION

In this paper, we studied the switching in Fe/MgO/Fe switching. It has been shown that the nearly half metallic nature of the Fe contacts results in a very asymmetric parallel to anti-parallel and parallel to anti-parallel switching profile.

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