Spin and Charge Drift-Diffusion Approach to Torque Computation in Magnetic Tunnel Junctions

Simone Fiorentini[1,*], Johannes Ender[1,2], Roberto L. de Orio[2],
Siegfried Selberherr[2], Wolfgang Goes[3], and Viktor Sverdlov[1,2]
[1] Christian Doppler Laboratory for Nonvolatile Magnetoresistive Memory and Logic
at the [2]Institute for Microelectronics, TU Wien, Gußhausstraße 27-29, A-1040 Wien, Austria
[3] Silvaco Europe Ltd., Cambridge, United Kingdom
*Email: fiorentini@iue.tuwien.ac.at

***Abstract*—As the interest in spin-transfer torque magnetoresistive memories for embedded and stand-alone applications is growing, reliable simulation tools are needed to help design and improve these devices. In this paper, we present a finite element implementation of the drift-diffusion approach for coupled spin and charge transport, commonly applied in metallic valves, to compute the torques acting in a magnetic tunnel junction which constitutes the cell of modern spin-transfer torque memories. We investigate the dependence of the torques on system parameters and demonstrate that it is possible to employ the drift-diffusion approach to reproduce the torque magnitude expected in magnetic tunnel junctions. We further show that a full 3D solution of the equations is necessary in order to accurately model the torques acting on the magnetization. The use of a unique set of equations for the whole memory cell constitutes the basis of an efficient finite element based approach to rigorously describe the switching process of novel spin-transfer torque memories.**

Keywords—Spin and charge drift-diffusion, spin-transfer torque, magnetic tunnel junctions, STT-MRAM

I. Introduction

Spin-transfer torque magnetoresistive random access memory (STT-MRAM) represents an emerging solution to the increased stand-by power consumption and leakages of CMOS devices. It is suitable for IoT and automotive applications, as well as for embedded DRAM and last level caches [1]-[7]. Improvements in the design of modern STT-MRAM devices are supported by the development of accurate simulation tools. The dynamics of the magnetization can be described by the Landau-Lifshitz-Gilbert (LLG) equation

$$\frac{\partial \mathbf{m}}{\partial t} = -\gamma\mu_0 \mathbf{m}\times\mathbf{H}_{\text{eff}} + \alpha\mathbf{m}\times\frac{\partial \mathbf{m}}{\partial t} + \frac{1}{M_S}\mathbf{T_S}, \qquad (1)$$

where $\mathbf{m}=\mathbf{M}/M_S$ is the position-dependent normalized magnetization, M_S is the saturation magnetization, α is the Gilbert damping constant, γ is the gyromagnetic ratio, μ_0 is the vacuum permeability, and $\mathbf{H}_{\text{eff}}$ is the effective magnetic field, containing various contributions such as the external field, the exchange interaction, the anisotropy field, and the demagnetizing field.

Modeling of STT switching can be performed by assuming a Slonczewski-like torque expression [8]

$$\mathbf{T_S} = \gamma\frac{\hbar}{2e}\frac{J_C\,P_{RL}}{d(1+P_{FL}P_{RL}\cos\theta)}\mathbf{m}\times(\mathbf{m}\times\mathbf{x}), \qquad (2)$$

where $\hbar$ is the reduced Plank constant, e is the electron charge, J_C is the current density, d is the thickness of the free layer, P_{FL} and P_{RL} are the polarizations of the free (FL) and reference layer (RL), respectively, θ is the angle between magnetization vectors in the FL and RL, and $\mathbf{x}$ is the magnetization direction of the RL. This approach, however, permits to only simulate the dynamics of a thin free layer. A more complete description of the process is achieved by computing the spin accumulation $\mathbf{S}$ across the whole structure.

II. Spin Drift-Diffusion Equations

The drift-diffusion equations for the spin accumulation and the resulting expression for the torque acting on the magnetization are

$$\mathbf{J_S} = \frac{\mu_B}{e}\beta_\sigma\left(\mathbf{J_C} + \beta_D D_e\frac{e}{\mu_B}[(\nabla\mathbf{S})\mathbf{m}]\right)\otimes\mathbf{m} - D_e\nabla\mathbf{S}, \qquad (3a)$$

$$\frac{\partial\mathbf{S}}{\partial t} = -\nabla\mathbf{J_S} - D_e\left(\frac{\mathbf{S}}{\lambda_{sf}^2} + \frac{\mathbf{S}\times\mathbf{m}}{\lambda_J^2} + \frac{\mathbf{m}\times(\mathbf{S}\times\mathbf{m})}{\lambda_\varphi^2}\right), \qquad (3b)$$

$$\mathbf{T_S} = -\frac{D_e}{\lambda_J^2}\mathbf{m}\times\mathbf{S} - \frac{D_e}{\lambda_\varphi^2}\mathbf{m}\times(\mathbf{m}\times\mathbf{S}), \qquad (3c)$$

where μ_B is the Bohr magneton, β_σ and β_D are spin polarization parameters, D_e is the electron diffusion

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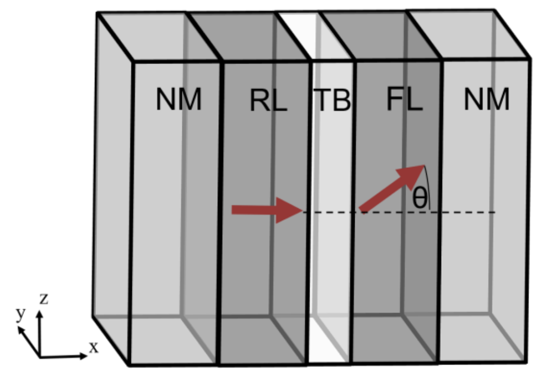

Fig. 1. MTJ structure used in the finite element simulations. The magnetization in the RL is fixed, the one in the FL is free to switch. NM are non-magnetic contact layers.

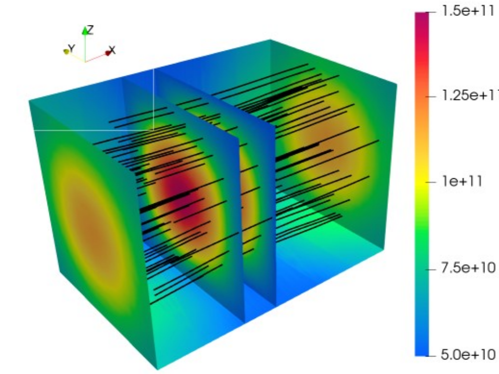

Fig. 2. Current density magnitude obtained for non-uniform magnetization configuration in the FL. The current is highly redistributed at the tunnel barrier interface to accommodate the varying resistance.

coefficient, λ_{sf} is the spin-flip length, λ_J is the exchange length, and λ_φ is the spin dephasing length.

This formalism has been successfully applied to metallic spin-valves with a non-magnetic spacer layer by solving the spin and charge drift-diffusion equations [9],[10]. The core element of modern STT-MRAM devices is, however, a magnetic tunnel junction (MTJ), with a tunnel barrier (TB) between the ferromagnetic layers (FM). The drift-diffusion approach thus must be extended to reproduce the torque expected in MTJs. The strong dependence of the large resistance on the relative magnetization vector orientation in the FL and the RL, described by the tunneling magnetoresistance ratio (TMR), can be reproduced by modeling the tunnel layer as a poor conductor with a low conductivity which incorporates the expected angular dependence [11]. This permits to obtain the electric current $\mathbf{J_C}$ entering (3a). The obtained current density, computed in the structure showcased in Fig. 1 for non-uniform FL magnetization configuration, parallel in the center and anti-parallel on the sides, is reported in Fig. 2.

We investigate the dependence of the average value of the damping-like torque in the FL on various system parameters, in order to calibrate our approach and reproduce the value predicted by Slonczewski. To compute the spin accumulation, we employ a Finite Element (FE) solver, implemented with the open source library MFEM [12].

III. Simulation results

We carried out simulations with a uniform magnetization along the x-direction in the RL and in the z-direction in the FL. Fig. 3 shows the dependence of the torque on the exchange length and on the diffusion coefficient D_S of the tunnel layer. In this approach D_S is a parameter to be chosen properly in order to reproduce the behavior of the spin accumulation and torques in an MTJ. The torque is very small at low values of D_S, while high values enhance the torque, as the slope of $\mathbf{S}$ reduces to the point of being practically preserved across the barrier. The torque is also enhanced by a lower value of λ_J, as in this case the transverse components of the spin accumulation are

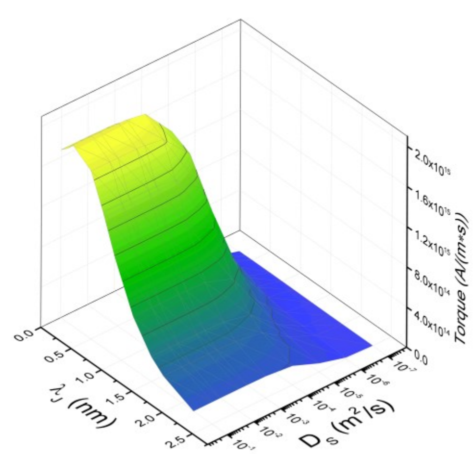

Fig. 3. Dependence of the torque on the exchange length and on the diffusion coefficient of the TB.

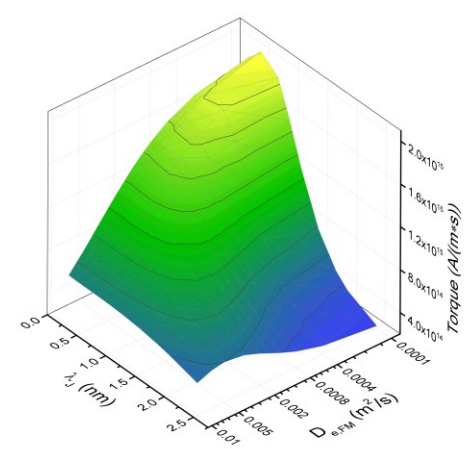

Fig. 4. Dependence of the torque on the exchange length and on the diffusion coefficient of the FM layers.

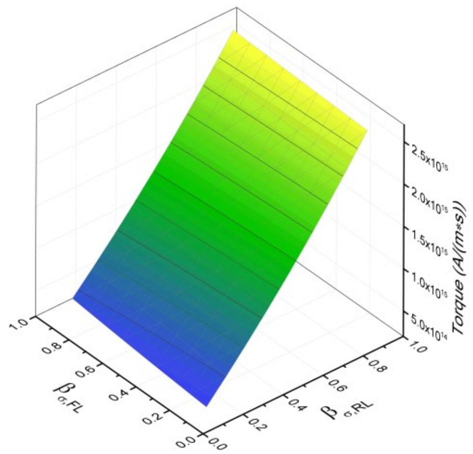

Fig. 4. Dependence of the torque on the polarization of the FL and the RL.

TABLE I. PARAMETERS

Parameter	Value
β_σ	0.7
β_D	0.8
$D_{e,NM}$	1x10^{-2} m^2/s
$D_{e,FM}$	1x10^{-4} m^2/s
D_S	5x10^{-1} m^2/s
λ_{sf}	10 nm
λ_J	0.5 nm
λ_φ	5 nm

completely absorbed in the space of the FL. Fig. 4 reports the dependence on the diffusion coefficient of the FM layers, $D_{e,FM}$, and on λ_J. The interplay between these two parameters is such that a lower $D_{e,FM}$ both enhances the torque and makes it more dependent on the exact value of the exchange length. The dependence on the polarization parameters $\beta_{\sigma,FL}$ and $\beta_{\sigma,RL}$ of the FL and RL, respectively, was also investigated. The results are reported in Fig. 4. The value of the torque in the FL mainly depends on the polarization of the RL, while it is almost constant with respect to the one of the FL, for every value of $\beta_{\sigma,RL}$. This suggests that, in our approach, these parameters are analogous to the current polarization entering the Slonczewski expression.

With the choice of parameters given in Table 1, we obtain a torque magnitude of $2.02 \cdot 10^{15}\ \mathrm{A/(m \cdot s)}$, compatible with the one computed with the Slonczewski approach (2) of $2.03 \cdot 10^{15}\ \mathrm{A/(m \cdot s)}$. The drift-diffusion approach is thus able to reproduce the torque magnitude expected in magnetic tunnel junctions. It also permits to compute the torque acting both on the FL and the RL. In Fig. 5, the spin accumulation and torque computed by the FE solver are compared to an analytical solution, obtained by extending the results presented in [13] to a multi-layered structure, showing that our results are in perfect agreement.

The main advantage of the FE implementation is the possibility to compute $\mathbf{S}$ with non-uniform magnetization configurations, typical for switching in complex structures. Thus, we investigate the difference between combining analytical solutions for the magnetization orientation at various y- and z-coordinates and computing the full 3D solution (Fig. 6). We compute the torque for the same magnetization configuration employed for the evaluation of $\mathbf{J_C}$. It can be seen that the first approach fails to account for the redistribution of $\mathbf{S}$ due to local gradients in the magnetization, such that the full solution computed by the FE solver is mandatory in order to properly model the torque acting on the magnetization.

IV. CONCLUSION

We employed a finite element implementation of the drift-diffusion approach for the computation of the torques acting in

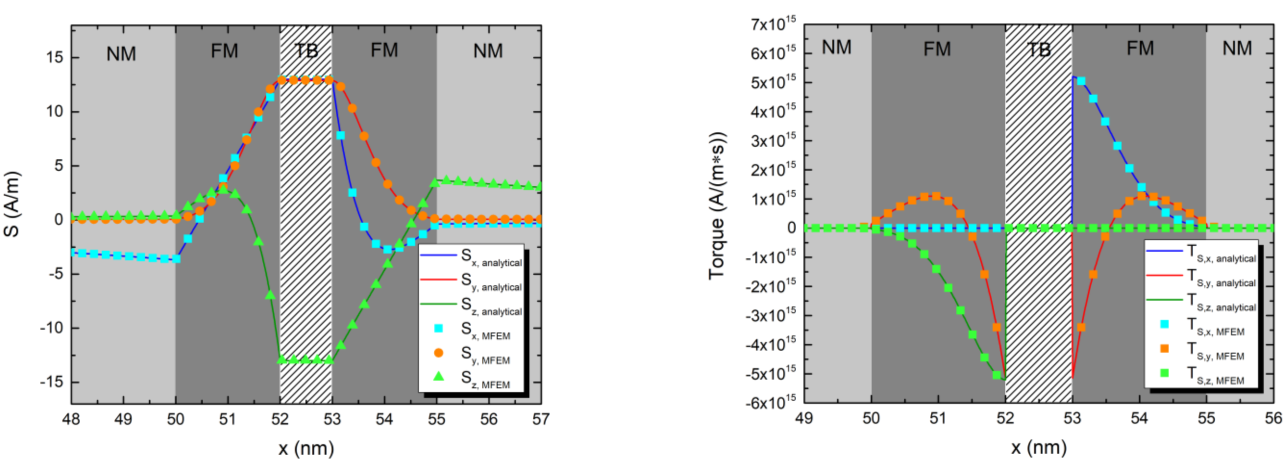

Fig. 5 Comparison of the spin accumulation (left) and torque (right) computed analytically and with the FE solver.

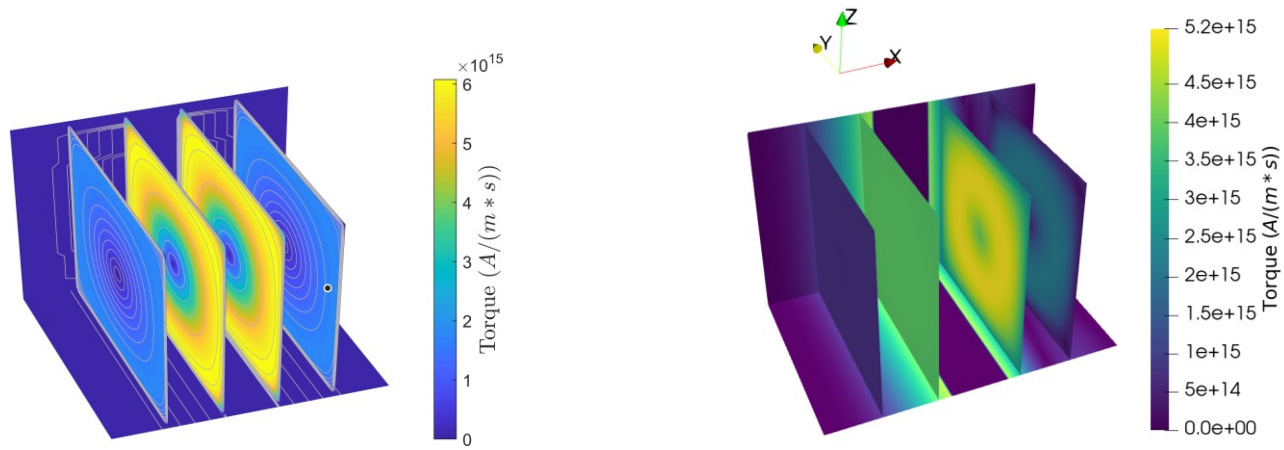

Fig. 6 Torque obtained combining multiple analytical solutions (left) compared to the one obtained by the FE solver (right).

a magnetic tunnel junction. We investigated the dependence of the spin-transfer torque on system parameters, and showed that our approach can reproduce the torque magnitude expected in a magnetic tunnel junction. Furthermore, we compared the finite element results with a known analytical solution, which was optimally reproduced by the solver. Finally, we showed that a full 3D solution is necessary in order to properly account for the redistribution of the torque due to local gradients of the magnetization. The drift-diffusion solver can then be applied to determine the magnetization dynamics in modern STT-MRAM devices.

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