First-principles Modeling of Magnetic Memory Components — Preliminary Results on the Effects of Interface Oxides

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ABSTRACT

We present preliminary results of our studies of the effects of oxides in the Fe/MgO interface of an Fe-MgO-Fe magnetotunnel junction. Specifically, we report on a significant decrease in calculated tunneling magnetoresistance when oxides are included, as well as a complete reduction of spin-current polarization for the parallel spin configuration when NiO is present.

Keywords: spintronics, magnetotunnel junction, tunneling magnetoresistance, interface layer, interface oxide, magnetic random access memory

1 INTRODUCTION

A theoretical understanding of magnetotunnel junctions (MTJs) currently plays a pivotal role in the development of new generations of hard disk drive read heads and novel spintronic devices, such as magnetic random access memory (MRAM).

MTJs with amorphous Al_2O_3 barriers were studied in the late 1990s [1], [2], and the fully crystalline Fe-MgO-Fe MTJ recently emerged as a "generic" research system [3]–[6]. This component is theoretically predicted to provide a tunneling magnetoresistance (TMR) in excess of 1000% [3], while TMR of up to 180% has been measured at room temperature [6].

The introduction of a single FeO layer in the Fe/MgO interface of such structures [7], [8], which can develop due to oxidation of the Fe electrode during structure growth, is known to reduce TMR significantly [9], [10][1]. NiFe and CoFeB electrodes are sometimes used to reduce the coercivity for low field operation [11] and to enhance TMR [12]–[14], respectively, and Mn is often used for exchange bias [15]. In order to achieve good structural quality annealing is often required, and as a result Ni, Co, and Mn diffuse into the interface and form NiO, CoO, and MnO.

This article describes preliminary results of our numerical studies of electron transport in an Fe-MgO-Fe MTJ. We have modeled this system with four different oxides in the Fe/MgO interface, and have studied to what extend different oxides influence TMR.

[1]Different FeO compositions (FeO, Fe_2O_3, and Fe_3O_4) can develop, so the TMR changes significantly from device to device.

2 MODEL

In earlier work [16], [17] we have modeled the zero-bias electron transport properties of Fe-MgO-Fe using the combination of density functional theory (DFT) and non-equilibrium Green's functions (NEGFs) implemented in the commercially available *Atomistix ToolKit* [18], [19]. In this work, we have used the latest version of this software (version 2.1).

The structure we have studied is shown in Figure 1, and is based on an experimental analysis of the atomic positions in such systems [8]. It includes 5 atomic layers

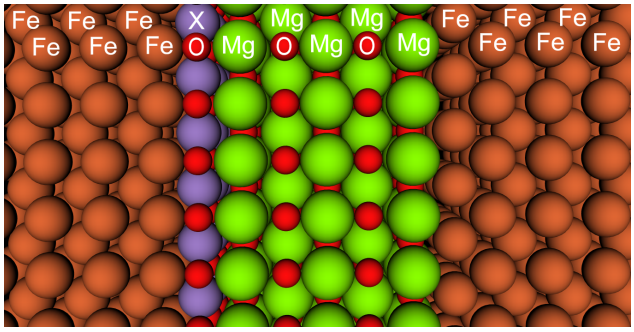

Figure 1: The generic structure under investigation. For systems including the interface oxides FeO, NiO, CoO, and MnO, X is Fe, Ni, Co, and Mn, respectively, and the left-most Oxygen atom is included; for the system without an interface layer, X is Fe and the Oxygen atom is excluded.

of MgO, and has been modeled with and without an oxide layer in the Fe/MgO interface (FeO, NiO, CoO, or MnO). In all calculations, the lattice constant of the Fe electrodes was held fixed at $a = 2.866$ Å; the atomic coordinates are detailed in earlier work [17].

The different oxide layers were incorporated in the structure by simple substitution of the right-most Fe atom in the left electrode of an Fe-FeOMgO-Fe system with Ni, Co, or Mn; the detailed structure of the "original" FeO layer is found in [8]. The structures were not relaxed after substitution, *i.e.* the systems were probably not in their minimum energy configurations.

The SCF calculations were converged to a tolerance of 10^{-6} using the SGGA exchange-correlation potential

[20]; the SZP basis set was used for Fe, while DZP basis sets were used for all other elements; a mesh-cutoff of 350 Rydberg was used. We used an 8×8 k-point mesh in the plane parallel to the interface for calculating the density matrix, 100 k-points in the transport direction, an electron temperature of 1 mK, and 100 points on the complex energy contour integral with a lower bound of -10 Rydberg [18].

The conductance calculations were performed by calculating the zero-bias transmission at the Fermi energy using 90,601 k-points, equally distributed in the Brillouin zone parallel to the interface. As mentioned in [16], an extremely large number of k-points must be used to ensure convergence for the minority-spin conductance in transmission calculations, while the majority-spin calculations are well converged using only a limited number of k-points. Mathon and Umerski find that 10^6 k-points are needed to converge the minority-spin calculations [3], but we find that 301×301 k-points provide a reasonable balance between accuracy and calculation time. The results for minority-spin should, however, be regarded with caution.

Based on extensive convergence studies and other available information, we estimate the accuracy of calculated TMR to be on the order of $\pm 20\%$.

3 RESULTS

The zero-bias conductance was calculated for all five systems in the parallel- and anti-parallel configurations, and the resulting TMR was found from

$$R_{TMR} \equiv \frac{R_{AP} - R_P}{R_P}, \tag{1}$$

where R_P and R_{AP} are the resistances for parallel- and anti-parallel configurations, respectively, *i.e.* the inverse of the corresponding zero-bias conductances.

The calculated values of the TMR are listed in Table 1 and plotted in Figure 2.

	$R_P \cdot A$	$R_{AP} \cdot A$	R_{TMR}	P_P	P_{AP}
No IL	1.40	25.9	1754%	83%	-1%
FeO	165	410	148%	79%	-76%
NiO	109	130	19%	1%	-87%
CoO	135	628	363%	94%	-58%
MnO	117	606	419%	91%	-35%

Table 1: Calculated TMR for the structures with different interface layers (IL) shown in Figure 1, along with the resistance-area product, $R \cdot A$, (in units of $\Omega\,\mu\text{m}^2$) and the polarization of the spin-current, P. Results for parallel- and anti-parallel spin configurations are listed.

Clearly, the introduction of an interface oxide significantly decreases the TMR, and apparently the effect of

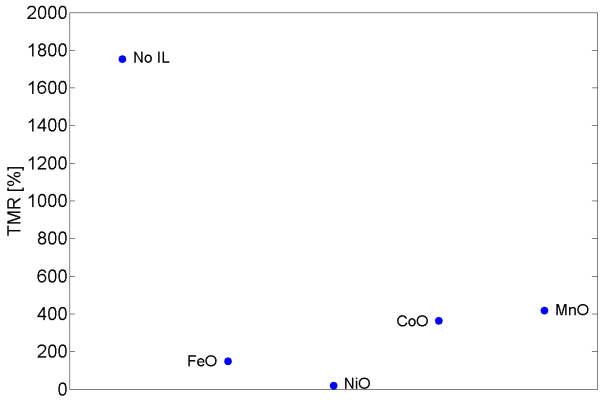

Figure 2: Calculated TMR of the Fe-MgO-Fe MTJ with different interface layers (IL).

NiO is greater than that of CoO and MnO, while the effect of FeO is somewhere in between.

Also listed in Table 1 is the resistance-area product, $R \cdot A$, and the polarization of the spin-current, defined

$$P \equiv \frac{G_\uparrow - G_\downarrow}{G_\uparrow + G_\downarrow}, \tag{2}$$

where $G_\uparrow$ and $G_\downarrow$ are the spin-up and -down conductances, respectively. It is obvious that the "generic" Fe-MgO-Fe MTJ works as a spin filter when in the parallel configuration, polarizing the spin-current, and that NiO — as the only interface layer — strongly reduces this effect. For the anti-parallel spin configuration, the "generic" system shows negligible polarization[2], while all remaining systems (including the NiO system) show medium- to large negative polarization. It is also obvious that the interface oxides increase the resistance of the device for both configurations of the spin, most significantly for the parallel configuration (hence the decrease in TMR).

4 CONCLUSIONS AND PERSPECTIVES

We have calculated the zero-bias conductance for parallel- and anti-parallel configurations of the electrode spins for an Fe-MgO-Fe magnetotunnel junction with four different interface oxide layers, as well as without such layers.

We find that the resulting tunneling magnetoresistance decreases significantly for systems including such

[2]Due to the mirror symmetry of the "generic" system, an electron with spin-up will have as much probability of tunneling from the left electrode to the right as a spin-down electron will have of tunneling in the opposite direction (and *vice versa*). The polarization is therefore zero.

oxide layers, and that the effect is most significant for NiO, for which the tunneling magnetoresistance is close to zero. We also find that the polarization of the spin-current, which is $\approx 85\%$ for most systems in the parallel spin configuration, is negligible when NiO is present, while the polarization is negative for all oxide systems (including NiO) in the anti-parallel configuration.

We are currently looking into the underlying physical phenomena causing these effects, and expect to report in detail soon.

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