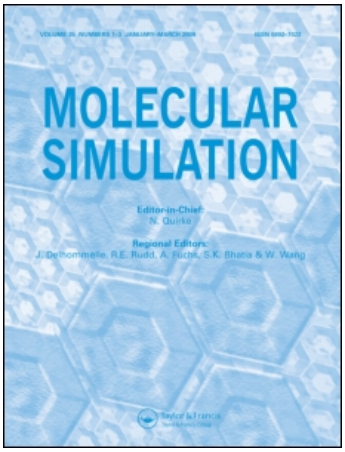

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Crystalline magnetotunnel junctions: Fe-MgO-Fe, Fe-FeOMgO-Fe and Fe-AuMgOAu-Fe

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We have modeled the electrical properties of three magnetotunnel junctions (MTJs) using a density functional theory (DFT), non-equilibrium Green's functions (NEGFs) based commercial code. We find results similar to those in the literature, and propose investigations into the effects of perturbations to the exact positions of the atoms in these structures.

Keywords: Spintronics; Magnetotunnel junction; Magnetic random access memory; MRAM; Electron transport

1. Introduction

A detailed understanding of magnetotunnel junctions (MTJs) of high magnetoresistance (MR) is highly beneficial for the development of magnetic random access memory (MRAM) and other novel devices.

MTJs with amorphous Al_2O_3 barriers have been studied [1,2], but these devices show only limited MR, and are virtually impossible to model due to the non-crystalline structure of the oxide. Fully crystalline MTJs with MgO barriers currently appear interesting for research and possible development.

MgO has been successfully grown on Fe(001) using molecular beam epitaxy (MBE) [3], and Fe-MgO-Fe devices of good structural quality have been grown by MBE and pulsed laser deposition (PLD) [4]. The electrical properties of such Fe-MgO-Fe devices have been studied using first-principles- and tight-binding methods [5,6], and tunneling magnetoresistances (TMRs) in excess of 1000% have been predicted [6].

The top-most atomic layer of the Fe substrate, unfortunately, seems to oxidize during MgO growth, and an atomic layer of FeO probably exists at the Fe-MgO interface in such devices [7,8], although Fe-MgO-Fe can probably be grown without such a layer [9]. These FeO layers have a very significant effect on the electrical properties of the devices [10], and the TMR is predicted to be much smaller for Fe-FeOMgO-Fe devices than for Fe-MgO-Fe devices [10,11].

To avoid the oxidation of the top-most Fe layer, one could imagine growing a thin layer of Au on the Fe substrate before growth of MgO. Including a Au layer at the top MgO-Fe interface, to make the structure symmetric, such Fe-AuMgO-Fe devices are predicted to possess TMR in excess of 1000% [12], and are therefore interesting for future MRAM devices.

This article describes a preliminary study of the electrical properties of Fe-MgO-Fe, Fe-FeOMgO-Fe and Fe-AuMgOAu-Fe structures.

2. Model

We have modeled the zero-bias transmission properties of Fe-MgO-Fe (structure I), Fe-FeOMgO-Fe (structure II) and Fe-AuMgOAu-Fe (structure III) using the commercially available *Atomistix ToolKit* [13,14] (version 2.0), which is based on density functional theory (DFT) and non-equilibrium Green's functions (NEGFs). The structures, shown in figure 1, were based on the coordinates given in [8], and include five atomic layers of MgO; the lattice constant of the Fe electrodes was held fixed at $a = 2.866$ Å.

The properties were calculated at the Fermi energy using 40,401 k-points, equally distributed in the Brillouin zone parallel to the interfaces, and at the k-point $(k_x, k_y) = (0, 0)$ using 401 equally spaced energy points. The SCF calculations were converged to a tolerance of 10^{-6} using the SGGA exchange-correlation potential [15], DZP basis

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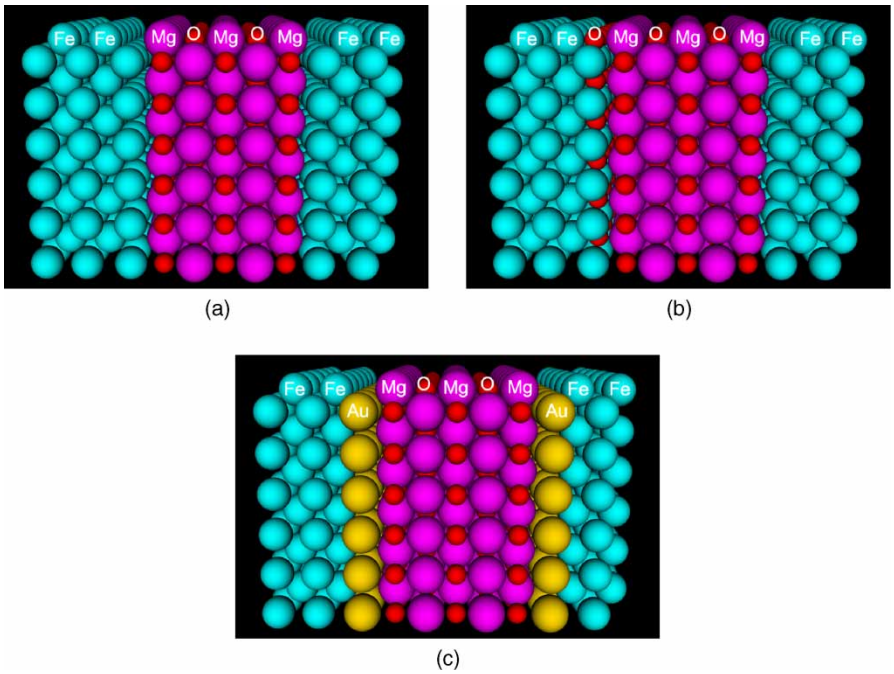

Figure 1. The three structures, (a) Fe-MgO-Fe (structure I), (b) Fe-FeOMgO-Fe (structure II) and (c) Fe-AuMgOAu-Fe (structure III). Note the FeO layer in the Fe/MgO interface of Fe-FeOMgO-Fe and the Au layers in the Fe/MgO and MgO/Fe interfaces of Fe-AuMgOAu-Fe.

sets for all elements, and a mesh-cutoff of 150 Rydberg. We used an 8×8 k-point mesh in the plane parallel to the interfaces and an electron temperature of 0.1 eV. The results of the calculations are discussed briefly below.

3. Results

3.1 *Convergence of k*-point sampling

The relative conductances of the Fe-MgO-Fe structure—calculated at the Fermi energy for a number of k-point "resolutions", in the range $(21 \times 21), (31 \times 31), \ldots, (201 \times 201)$, and normalized by the result found using (201×201) k-points—are shown in figure 2.

It is clear that the majority-spin conductance calculation is well converged when using (201×201) k-points, while the minority-spin calculation is not converged. This difference is expected, since the transmission occurs through different mechanisms for the two spin-orientations, as described below. Sampling at (201×201) k-points is quite time-consuming, and it has therefore not been feasible to sample using more k-points in this study; the quantitative results, presented in Section 3, should therefore be regarded with caution. Since the minority-spin transmission is similar in nature for all three structures, it must be assumed that this goes for all three, albeit this convergence analysis has only been performed for Fe-MgO-Fe.

3.2 *Qualitative results of* $\vec{k}_{\|}$*-resolved transmission calculations*

The $\vec{k}_{\|}$-resolved transmission spectra for majority-spin electron transport at the Fermi energy, shown in figure 3, look qualitatively very similar for the three systems: The transmission occurs through Bloch states with wavevectors near $(k_x, k_y) = (0, 0)$. The spectra correspond nicely with

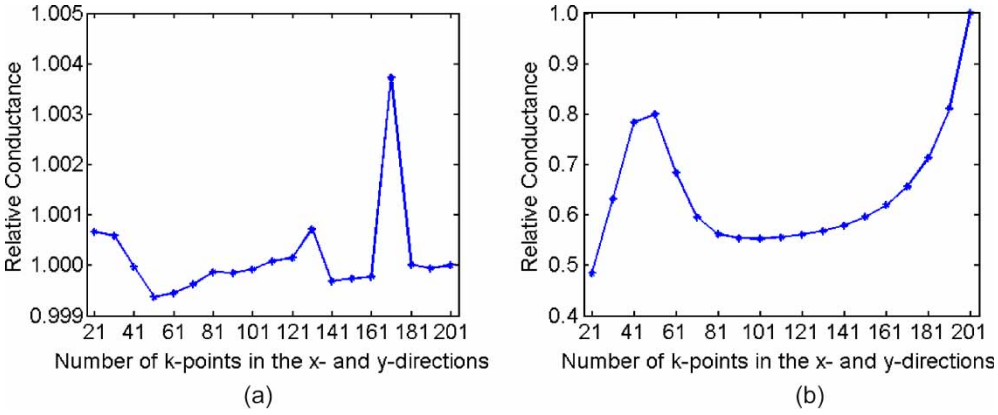

Figure 2. Relative conductance, calculated with different k-point "resolutions", for (a) the majority-spin and (b) the minority-spin. The results have been normalized by the value found using (201 × 201) k-points.

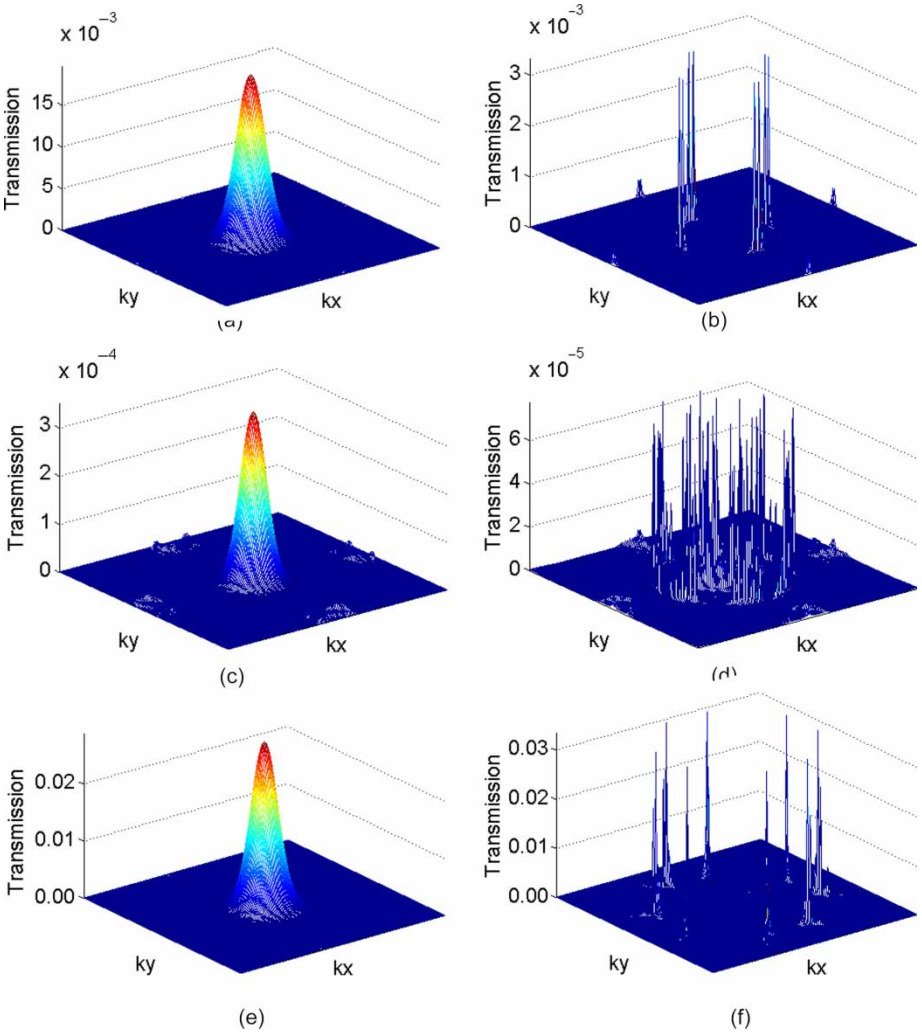

Figure 3. Majority- and minority-spin transmission at the Fermi energy for Fe-MgO-Fe (a and b), Fe-FeOMgO-Fe (c and d) and Fe-AuMgOAu-Fe (e and f).

the spectra found in the literature [5,6,11,12]; majority-spin transport seems to occur through simple barrier tunneling. The $\vec{k}_{\|}$-resolved transmission spectra for minority-spin transport at the Fermi energy, also shown in figure 3, also look qualitatively very similar for the three systems: All spectra show almost zero transmission in the two-dimensional Brillouin zone, except for some very sharp peaks at specific values of the wavevectors (this is the reason the minority-spin calculations are difficult to converge, cf. Section 1). The specific values are different for the three systems, but the overall "peaked transmission" is similar. The spectra correspond nicely with the spectra found in the literature [5,6,11,12]; minority-spin transport seems to occur through complex resonance tunneling.

3.3 Quantitative results of $\vec{k}_{\|}$-resolved conductance calculations

The conductances calculated using 201×201 k-points are listed in table 1, along with the relative differences in the conductances found for the majority- and minority-spin, represented by

$$\Delta G \equiv \frac{G_{\text{majority}} - G_{\text{minority}}}{G_{\text{minority}}}$$

The results show that the majority-spin conductance, G_{majority}, is much larger than the minority-spin conductance, G_{minority}, for the Fe-MgO-Fe system, while it is only slightly larger for the Fe-FeOMgO-Fe system. This is in correspondence with the results found in the literature [5,6,10]. It has been argued that the reason for the smaller value of ΔG for Fe-FeOMgO-Fe than for Fe-MgO-Fe is

Table 1. Calculated conductances for structures I–III in units of nS (10^{-9} Siemens), and the relative differences in the conductances for the majority- and minority-spins, $\Delta G \equiv (G_{\text{majority}} - G_{\text{minority}})/G_{\text{minority}}$.

	I	*II*	*III*
G_{majority}	14.3	0.201	19.7
G_{minority}	0.104	0.0130	1.46
ΔG	136	14.4	12.5

that the partial electron density of states for the majority-spin state Δ_1, which is the main contributor to the majority-spin conductance [5], is greatly reduced in the Fe/MgO interface by the introduction of the O atoms in the surface Fe layer [10]; the surface Fe atoms simply couple to the O atoms in the FeO layer rather than the O atoms in the MgO layer. This strongly reduces the majority-spin conductance, while the FeO layer only slightly reduces the minority-spin conductance, and thus brings down the value of ΔG.

For Fe-AuMgOAu-Fe, the majority-spin conductance is only slightly larger than the minority-spin conductance. The majority-spin conductance is roughly the same size as for Fe-MgO-Fe and Fe-FeOMgO-Fe, while the minority-spin conductance is large compared tothese structures. It has recently been argued that this large minority-spin conductance is mediated by quantum well states in the Au layers [12], and for thicker Au layers the minority-spin conductance is even predicted to become larger than the majority-spin conductance, in contrast to the results for Fe-MgO-Fe and Fe-FeOMgO-Fe discussed above.

3.4 Quantitative results of energy-resolved transmission calculations

The energy-resolved transmission spectra for majority-spin transport at the two-dimensional Γ-point are shown in figure 4.

The spectra show that Fe-MgO-Fe has finite transmission at the Fermi energy ($E = 0$), while Fe-FeOMgO-Fe has close to zero transmission at this energy. This cooperates the argument that the Δ_1 state, which has $(k_x, k_y) = (0, 0)$, is "de-coupled" by the FeO layer (cf. Section 3). The Fe-AuMgOAu-Fe spectrum shows finite transmission at the Fermi energy, and generally shows transmission somewhat similar to that for Fe-MgO-Fe (as expected).

Analogous transmission spectra have been calculated for the minority-spin, but these do not bring any relevant insight, since much more than a single k-point is needed to correctly model the minority-spin transport (cf. Section 1); they are not shown.

4. Conclusions and perspectives

We have modeled the electrical properties of three related MTJs, namely Fe-MgO-Fe, Fe-FeOMgO-Fe and Fe-AuMgOAu-Fe.

We find that a fine grid of k-points is necessary to correctly model minority-spin transport for such systems, while only a few k-points are necessary to model majority-spin transport. The minority-spin results in this article are not converged, since using a k-point sampling of more than (201×201) has not been computationally feasible, and should therefore be regarded with caution. By utilizing the symmetries of the system for increased performance, which is possible in the next version of the software employed, we expect to be able to increase the number of k-points in future studies, and in that way provide more accurate results for the minority-spin transmission and -conductance.

We also find, in correspondence with results found in the literature, that two different transport mechanisms

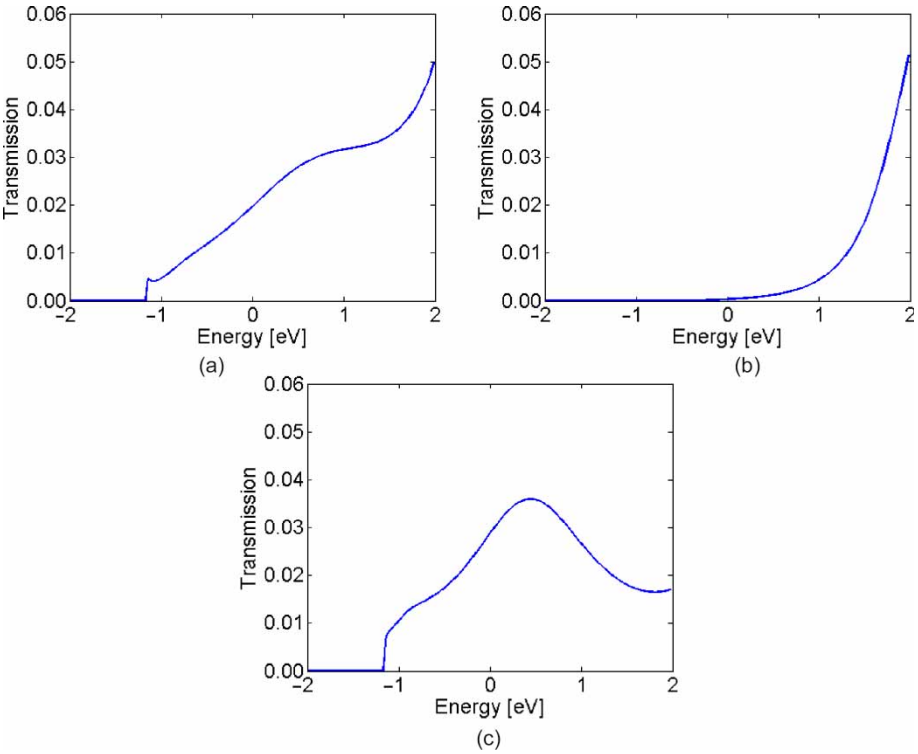

Figure 4. Majority-spin transmission with $(k_x, k_y) = (0, 0)$ for (a) Fe-MgO-Fe, (b) Fe-FeOMgO-Fe and (c) Fe-AuMgOAu-Fe.

are involved in the transport of majority- and minority-spin electrons: Majority-spin transport occurs through simple barrier tunneling, while minority-spin transport occurs through complex resonance tunneling. Further analysis of the transport mechanisms is described in [16].

Finally, we find—also in correspondence with results found in the literature—that the FeO layer in Fe-FeOMgO-Fe strongly reduces the majority-spin conductance, while only slightly reducing the minority-spin conductance. In contrast, the majority-spin conductance appears more or less unaffected by the introduction of a single Au layer in the two interfaces, while the minority-spin conductance is strongly enhanced. Transport through such Fe-AuMgOAu-Fe structures is not fully understood, and further investigations are planned.

In this work, we have modeled the electron transport properties of three related, but different, structures. Such studies can provide insight into the transport mechanisms of these systems, and can prove valuable in the design of novel spintronic devices, such as MRAM. We propose that further investigations of such structures be undertaken, and have developed plans to do so. Specifically, we plan investigations into the effects of small variations of the positions of the atoms in the structures, as the resonance tunneling of the minority-spin electrons is expected to by highly sensitive to such "perturbations". Even small changes in the atomic positions may have a large influence on the calculated conductances, and the "accuracy" of current numerical results can therefore not be assessed without such studies.

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