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Theory of resonant spin-dependent tunneling in an Fe/Ag/MgO/Fe(001) junction

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Calculation of the tunneling magnetoresistance (TMR) of an Fe/Ag/MgO/Fe(001) magnetic junction is reported. The magnetoresistance is determined without any approximations from the real-space Kubo formula using tight-binding bands fitted to an *ab initio* band structure. It is shown that the calculated TMR oscillates as a function of Ag interlayer thickness between positive values in excess of 2000% and negative values of the order of −100%. The oscillation period is determined by the spanning vector of the Ag Fermi surface. The large positive TMR and the changes in its sign are due to resonant enhancement of the tunneling conductance of majority-spin carriers in the ferromagnetic configuration and of the conductance of carriers tunneling in the antiferromagnetic configuration from the minority-spin channel in the Fe electrode adjacent to the Ag layer to the majority-spin channel in the other Fe electrode. The resonant enhancement occurs because the Ag interlayer creates potential steps for electrons in both the ferromagnetic and antiferromagnetic configurations of the junction. This mechanism, which results in a very large TMR, is quite different from the mechanism that causes large TMR in the standard Fe/MgO/Fe(001). It offers the possibility of tuning the magnitude and sign of the TMR by the choice of the interlayer thickness. A Lateral supercell method was also used to investigate the effect of interfacial roughness on the resonant tunneling in an Fe/Ag/MgO/Fe(001) junction. It is found that, in contrast to the Fe/MgO/Fe(001) junction whose TMR is reduced drastically by disorder, the junction with a silver interlayer is much less affected by interfacial roughness.

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I. INTRODUCTION

The observed magnitude of the tunneling magnetoresistance (TMR) in junctions with an MgO barrier now approaches the TMR ratio predicted theoretically[1,2] for a perfect Fe/MgO/Fe(001) junction with coherent tunneling. We can, therefore, conclude that tunneling in MgO junctions that are studied experimentally must be coherent. In an epitaxial junction with coherent tunneling the electron wave vector parallel to the layers $\boldsymbol{k}_{\parallel}$ is conserved. It follows that tunneling is determined by the matching of electron wave functions across the whole junction and, therefore, the TMR ratio depends critically on the particular combination and crystal orientation of the materials from which the junction is composed. This opens up the possibility of exploring composite MgO-based junctions with coherent tunneling whose properties can be engineered to suit applications. In particular, it should be possible to observe resonant tunneling in MgO-based junctions. This can occur for a double-barrier magnetic junction[3,4] and quantum oscillations of the tunneling conductance have already been observed in such a system.[5] Another possibility is to create quantum wells in an MgO-based junction by introducing two symmetric nonmagnetic interlayers which lead to resonant enhancement of the tunneling conductance in the ferromagnetic configuration of the junction.[6] However, it is difficult to grow epitaxial tunneling junctions with a relatively large number of layers of different materials. We, therefore, propose one way to fundamentally alter the properties of an MgO-based junction by inserting just a single nonmagnetic metallic interlayer between one of the magnetic electrodes and the MgO barrier. One might assume naively that nonmagnetic interlayers between the ferromagnetic electrodes and the barrier destroy the TMR effect since the surface density of states at the interface between the interlayer and tunneling barrier is spin independent. This argument would be valid for noncoherent tunneling where only the surface density of states at the interface with the barrier determines the TMR. However, we showed earlier[7] that TMR remains nonzero for coherent tunneling in a cobalt junction with vacuum gap when a copper interlayer is inserted between one of the Co electrodes and the gap. Our explanation of nonzero TMR was that a mismatch between electron bands in Co and Cu leads to the formation of resonant quantum-well (QW) states in the Cu interlayer. Since the mismatch is large only for minority-spin (down spin) electrons, QW states are formed predominantly in the down-spin channel. It follows that a large spin asymmetry in transport and, hence, nonzero TMR remains. This prediction was confirmed experimentally for a Co/Cu/$\mathrm{Al_2O_3}$/Py junction[8] in which the alumina barrier was amorphous. It should be noted that a finite TMR could be observed in this experiment, despite the fact that the barrier was amorphous since only coherence of transport in the Co/Cu bilayer is strictly required for nonzero TMR.[9] However, the TMR ratio for such a junction with an amorphous barrier was very small, of the order of several percent.[8]

We show here that coherence of transport across the whole junction with a nonmagnetic interlayer, which could be achieved in crystalline MgO-based junctions, results in resonant tunneling that can be exploited to control predictively not only the magnitude but even the sign of the TMR ratio. Suitable candidates for nonmagnetic interlayers are gold, silver, or copper. We consider here as an example an Fe/Ag/MgO/Fe(001) junction. Our calculations based on Kubo-Landauer formula using a fully realistic band structure predict that the TMR ratio in such a junction can be tuned between a positive TMR, well in excess of 2000%, and a

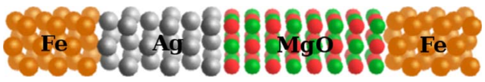

FIG. 1. (Color online) Schematic picture of the arrangement of atoms in Fe/Ag/MgO/Fe(001) junction.

negative TMR of the order of −100% by the appropriate choice of Ag and MgO thicknesses. It will be shown that the choice of a crystalline MgO barrier is crucial for such a tuning of the TMR resulting in very high TMR ratios although the quality of the Fe/Ag interface is relatively unimportant.

II. THEORETICAL FORMULATION

Measurements of the oscillatory exchange coupling in Fe/Ag/Fe(001) trilayers[10] show not only the long-period but even the short-period oscillation, which proves that near perfect coherence of electron wave functions can be achieved in this system for Ag interlayers as thick as 50 atomic planes.[10] These experiments also show that fcc Ag grows well on bcc Fe because of the small lateral mismatch to the Fe lattice. Similarly, the mismatch to the MgO rocksalt structure is also small. We, therefore, assume that the growth is pseudomorphic in the whole structure and neglect in our calculations any small lattice mismatch (roughness at the Fe/Ag interface will be included later). The way individual atomic planes of Fe, Ag, and MgO layers are arranged in the Fe/Ag/MgO/Fe(001) junction is shown schematically in Fig. 1. Details of the interface structure can be found in Ref. 6. We describe the band structure of the Fe electrodes and that of the Ag interlayer by tight-binding bands fitted to the *ab initio* band structure of bcc Fe and fcc Ag.[11] Similarly, the barrier is described by tight-binding bands fitted to the band structure of bulk MgO.[12] The on-site potentials in the Fe/Ag interface plane were adjusted self-consistently to preserve charge neutrality and to reproduce the correct surface moment of Fe. The band gap for the band structure of bulk MgO we use is 7.6 eV. Further details of our tight-binding parametrization may be found in Ref. 1.

The tunneling conductance Γ^σ in the spin channel σ of a Fe/Ag/MgO/Fe(001) junction was determined by the same method as in our previous calculation for Fe/MgO/Fe.[1] The tunneling current between two neighboring atomic planes in the MgO barrier, labeled 0 and 1, was evaluated from the real-space Kubo formula. Using a mixed representation, that is, Bloch-type in the plane of the layers and atomiclike in the perpendicular direction, it is easy to express the Kubo formula in terms of one-electron Green's functions at the Fermi surface ($E = E_F$). The conductance Γ^σ is given by

$$\Gamma^\sigma = \frac{4e^2}{h}\sum_{\boldsymbol{k}_\parallel} \mathrm{Tr}\{[\boldsymbol{T}_\sigma \,\mathrm{Im}\, \boldsymbol{G}_0^\sigma(\boldsymbol{k}_\parallel)]\,.\,[\boldsymbol{T}_\sigma^\dagger \,\mathrm{Im}\, \boldsymbol{G}_1^\sigma(\boldsymbol{k}_\parallel)]\}. \qquad (1)$$

The summation in Eq. (1) is over the two-dimensional (2D) Brillouin zone (BZ) and the trace is over the orbital indices corresponding to s,p,d orbitals that are required in a tight-binding parametrization of the junction. Finally, $\boldsymbol{G}_0^\sigma(\boldsymbol{k}_\parallel)$ and $\boldsymbol{G}_1^\sigma(\boldsymbol{k}_\parallel)$ are the one-electron Green's functions at the left (right) surfaces of a junction, that is, separated into two independent parts by an imaginary cleavage plane drawn between the atomic planes 0 and 1. The separation of the junction into two independent parts is made simply for calculational purposes and the conductance given by Eq. (1) is independent of the cleavage plane position. The junction remains physically connected and the interaction between the left and right parts is fully restored in Eq. (1) by the matrices $\boldsymbol{T}_\sigma$ and $\boldsymbol{T}_\sigma^\dagger$ defined by

$$\boldsymbol{T}_\sigma = \boldsymbol{t}_{01}(\boldsymbol{k}_\parallel)[\boldsymbol{I} - \boldsymbol{G}_1^\sigma(\boldsymbol{k}_\parallel)\boldsymbol{t}_{01}^\dagger(\boldsymbol{k}_\parallel)\boldsymbol{G}_0^\sigma(\boldsymbol{k}_\parallel)\boldsymbol{t}_{01}(\boldsymbol{k}_\parallel)]^{-1}, \qquad (2)$$

where $\boldsymbol{I}$ is a unit matrix in the orbital space and $\boldsymbol{t}_{01}(\boldsymbol{k}_\parallel)$ is the tight-binding hopping matrix connecting the surfaces 0 and 1. The calculation of the surface Green's functions and the problems of numerical accuracy are discussed in Ref. 1.

III. CALCULATED RESULTS FOR Fe/Ag/MgO/Fe(001) MAGNETIC TUNNELING JUNCTION

We are now ready to present our results for the Fe/Ag/MgO/Fe(001) junction obtained from the Kubo-Landauer formula (1). We use the "optimistic" tunneling magnetoresistance ratio $\mathrm{TMR} = (\Gamma_{\mathrm{FM}} - \Gamma_{\mathrm{AF}})/\Gamma_{\mathrm{AF}}$, where Γ_{FM} and Γ_{AF} are the total conductances in the ferromagnetic and antiferromagnetic configurations of the junction. The dependences of the magnetoresistance ratio on the thicknesses of Ag and MgO layers calculated from Eq. (1) are shown in Fig. 2(a). The dependences of the conductances $\Gamma^{\uparrow\uparrow}$ and $\Gamma^{\downarrow\downarrow}$ in the ferromagnetic and $\Gamma^{\uparrow\downarrow}$ and $\Gamma^{\downarrow\uparrow}$ in the antiferromagnetic configuration of the junction on Ag thickness are shown in Fig. 2(b) for a fixed MgO thickness of eight atomic planes. All the conductances are measured in units of the quantum conductance (e^2/h). Remarkably the TMR oscillates between positive and negative values as a function of Ag thickness with a period that is independent of MgO thickness. The amplitude of TMR oscillations increases with MgO thickness and the positive TMR in this system can reach several thousand percent. The large magnitude of TMR and the changes in its sign with Ag thickness occur because TMR is dominated just by two conductances, i.e., the conductance of majority-spin carriers in the ferromagnetic configuration $\Gamma^{\uparrow\uparrow}$ and the conductance $\Gamma^{\downarrow\uparrow}$ of carriers tunneling in the antiferromagnetic configuration from the minority-spin channel in the left Fe electrode (next to the Ag layer) to the majority-spin channel in the right Fe electrode. These two conductances oscillate as a function of Ag thickness with large comparable amplitudes and exhibit a phase shift which makes them oscillate almost in antiphase. To understand this behavior, the following questions have to be addressed. Why do the conductances $\Gamma^{\uparrow\uparrow}$ and $\Gamma^{\downarrow\uparrow}$ dominate, why do they oscillate with Ag layer thickness, and why is there a large phase shift between the oscillations of $\Gamma^{\uparrow\uparrow}$ and $\Gamma^{\downarrow\uparrow}$? To answer these questions, we first examine the distribution of the partial conductances $\Gamma^{\uparrow\uparrow}(\boldsymbol{k}_\parallel)$ and $\Gamma^{\downarrow\uparrow}(\boldsymbol{k}_\parallel)$ in the two-dimensional BZ. They are shown in Figs. 3 and 4 for the thickness of MgO of 15 atomic planes and two different thicknesses of Ag of 14 atomic planes (Fig. 3) and 16 atomic planes (Fig. 4). Figure 3, where the Ag thickness is 14 atomic planes, illustrates the situation when the conductance $\Gamma^{\downarrow\uparrow}$ is higher

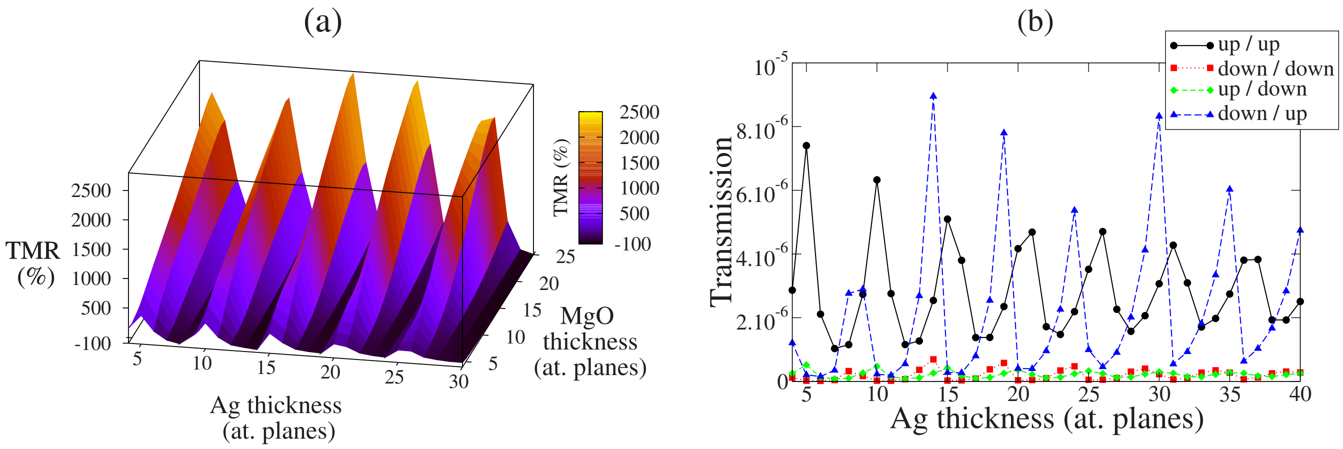

FIG. 2. (Color online) (a) TMR as a function of Ag and MgO thickness; (b) the individual conductances as a function of Ag thickness for a fixed MgO thickness of eight atomic planes.

than $\Gamma^{\uparrow\uparrow}$ and the TMR ratio is negative. It can be seen from Fig. 3(b) that this is due to a resonant enhancement of $\Gamma^{\downarrow\uparrow}$ which occurs on a small ring in the $\boldsymbol{k}_{\parallel}$ space centered around $\boldsymbol{k}_{\parallel}=0$ (the Γ point). At the same time, the conductance $\Gamma^{\uparrow\uparrow}$ remains unenhanced. The situation depicted in Fig. 4 for Ag thickness of 16 atomic planes is just the opposite. The conductance $\Gamma^{\uparrow\uparrow}$ is resonantly enhanced at the Γ point while $\Gamma^{\downarrow\uparrow}$ is nonresonant. The corresponding TMR ratio is thus positive and very large. On the basis of these results, we propose that large-amplitude oscillations of $\Gamma^{\uparrow\uparrow}$ and $\Gamma^{\downarrow\uparrow}$ are due to resonant enhancement of the tunneling conductance by the Ag interlayer which creates potential wells or steps adjacent to the MgO barrier. The conductances $\Gamma^{\downarrow\downarrow}$ and $\Gamma^{\uparrow\downarrow}$ are much smaller because tunneling to the down-spin channel in the right Fe electrode is inefficient due to the fact that there are no *sp*-like states in the minority-spin iron band at the Γ point. This is exactly the same argument that applies also to the simple Fe/MgO/Fe(001) junction without the Ag interlayer.[2]

To demonstrate resonant tunneling in the $\Gamma^{\uparrow\uparrow}$ and $\Gamma^{\downarrow\uparrow}$ channels, we plot in Fig. 5(a) the dependences of $\Gamma^{\uparrow\uparrow}(\boldsymbol{k}_{\parallel}^{0})$ and $\Gamma^{\downarrow\uparrow}(\boldsymbol{k}_{\parallel}^{0})$ on Ag thickness for a single $\boldsymbol{k}_{\parallel}^{0}$ at which a resonance occurs. This is the Γ point for $\Gamma^{\uparrow\uparrow}(\boldsymbol{k}_{\parallel})$ and any point on the small ring shown in Fig. 3(b) in the case of $\Gamma^{\downarrow\uparrow}$. Figure 5(a) shows oscillations with a constant amplitude and period of 5.3 atomic planes determined by the spanning vector of the Ag Fermi-surface belly. These two features prove resonant enhancement of the $\Gamma^{\downarrow\uparrow}$ and $\Gamma^{\uparrow\uparrow}$ conductances due to the presence of a silver interlayer. This is confirmed by the periodic behavior of the local density of states in silver at the Fermi level as a function of the silver layer thickness, which is shown in Fig. 6.

To clarify the origin of the resonant enhancement and, in particular, to explain the phase shift between the oscillations of $\Gamma^{\downarrow\uparrow}$ and $\Gamma^{\uparrow\uparrow}$, we need to determine the nature of the electron states that dominate tunneling in these two channels. This can be done following the argument constructed in Ref. 13. It is easy to show that Eq. (1) for the conductance Γ^{σ} can be written in the form

$$\Gamma^{\sigma}=\frac{2e^{2}}{h}\sum_{\boldsymbol{k}_{\parallel}}\mathrm{Tr}[t(E_F,\boldsymbol{k}_{\parallel})t^{\dagger}(E_F,\boldsymbol{k}_{\parallel})], \tag{3}$$

where t is the transmission matrix and the trace is again over the orbital indices. It was shown in Ref. 13 that the matrix $tt^{\dagger}$ is Hermitian, its eigenvalues lie in the interval [0,1], and they determine the transmission probability of different conductance channels. The corresponding eigenvectors determine the orbital decomposition of the conductance channels. Such an analysis at the Γ point shows that there is only one nonzero eigenvalue both for $\Gamma^{\uparrow\uparrow}$ and $\Gamma^{\downarrow\uparrow}$. This implies that there is a single conductance channel which determines the conductances $\Gamma^{\uparrow\uparrow}$ and $\Gamma^{\downarrow\uparrow}$ in the vicinity of the Γ point. The orbital decomposition of this single conductance channel for $\Gamma^{\uparrow\uparrow}$ and $\Gamma^{\downarrow\uparrow}$ is shown in Fig. 7. It can be seen that in the case of $\Gamma^{\uparrow\uparrow}$, the conductance is via *spd*-like states in the left and

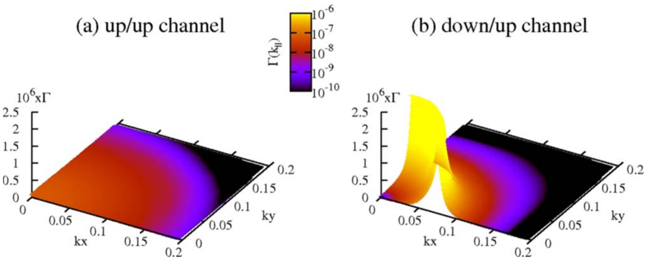

FIG. 3. (Color online) (a) Partial conductance $\Gamma^{\uparrow\uparrow}(\boldsymbol{k}_{\parallel})$ and (b) partial conductance $\Gamma^{\downarrow\uparrow}(\boldsymbol{k}_{\parallel})$ for Ag thickness of 14 atomic planes. Note that the BZ edges are at $k_x=\pm1$ and $k_y=\pm1$.

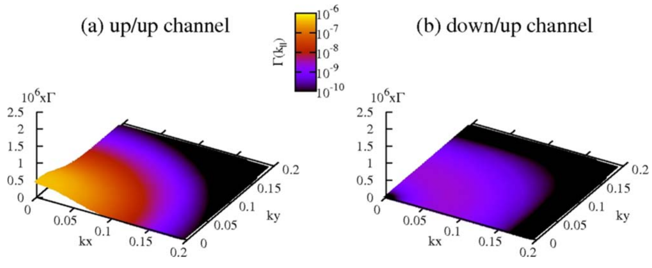

FIG. 4. (Color online) (a) Partial conductance $\Gamma^{\uparrow\uparrow}(\boldsymbol{k}_{\parallel})$ and (b) partial conductance $\Gamma^{\downarrow\uparrow}(\boldsymbol{k}_{\parallel})$ for Ag thickness of 16 atomic planes. Note that the BZ edges are at $k_x=\pm1$ and $k_y=\pm1$.

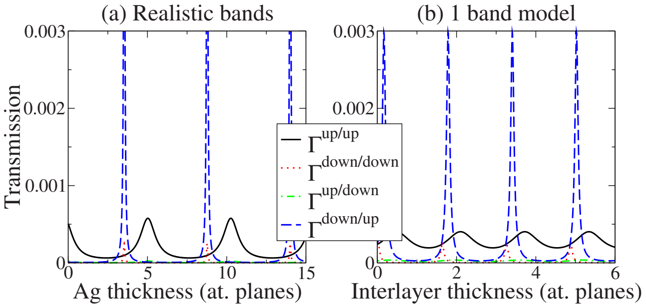

FIG. 5. (Color online) Dependences of $\Gamma^{\uparrow\uparrow}(\boldsymbol{k}_{\|}^{0})$ and $\Gamma^{\downarrow\uparrow}(\boldsymbol{k}_{\|}^{0})$ at a resonant point $\boldsymbol{k}_{\|}^{0}$ on Ag thickness: (a) fully realistic bands; (b) single-orbital model.

right Fe electrodes and also in the Ag interlayer. As expected, only *sp*-like states mediate tunneling through MgO. The fundamental difference, which occurs for $\Gamma^{\downarrow\uparrow}$, is that only a *d*-like state contributes in the left Fe electrode (minority-spin band). However, the orbital decomposition shows that the *d* state involved has the same rotational symmetry about the Γ point in the two-dimensional Brillouin zone as an *s*-like state. It follows that $\Gamma^{\uparrow\uparrow}$ and $\Gamma^{\downarrow\uparrow}$ in the left electrode have the same symmetry. The only difference is that the band width for minority-spin electrons in the left Fe electrode is much narrower than in the rest of the junction. The symmetry of the *d* state in the left Fe electrode explains the origin of the ring in the partial conductance $\Gamma^{\downarrow\uparrow}(\boldsymbol{k}_{\|})$ shown in Fig. 3(b). Tunneling from the *d* state is forbidden at the Γ point but allowed in its vicinity. Since perpendicular tunneling is favored, the competition between these two factors combined with the aforementioned symmetry of the *d* state involved results in a small ring in the conductance $\Gamma^{\downarrow\uparrow}(\boldsymbol{k}_{\|})$.

Since only a single conduction channel exists in the vicinity of the Γ point and the states mediating the conductance have the same symmetry in every part of the junction, we can attempt to model the whole junction by a simple single-orbital model. We use the same nearest-neighbor hopping $t=1$ eV in all parts of the junction for majority-spin electrons but model the narrow minority-spin band in the left Fe electrode by a much smaller hopping of $t=0.1$ eV. MgO is modeled by a potential barrier of 3.5 eV and the Ag interlayer is modeled by a potential step of 0.7 eV. The results of such a modeling are reproduced in Fig. 5(b). Comparing Figs. 5(a) and 5(b), we conclude that a single-orbital model reproduces very well the results obtained from the fully realistic calculation [Fig. 5(a)]. There are two essential features of the single-orbital model that are required to obtain the correct phase shift and shape of the resonance peaks: the minority-spin band in the left Fe electrode needs to be narrow and the Ag interlayer must be modeled by a potential step rather than by a potential well. The phase shift is rather independent of the step height but using a potential well instead of a step would result in a phase jump resulting in a phase shift of wrong sign. The height of the potential step is directly related to the period of conductance oscillations and is thus determined by fitting to the correct period coming from the spanning vector of the Ag Fermi-surface belly. The height of the potential barrier we use to model MgO only influences the overall magnitude of the conductance but does not influence either the phase shift or the shape of the resonance peaks.

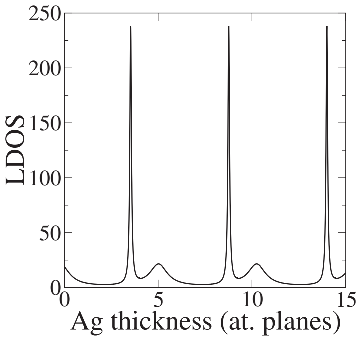

FIG. 6. Local density of states in silver at the Fermi level as a function of the interlayer thickness.

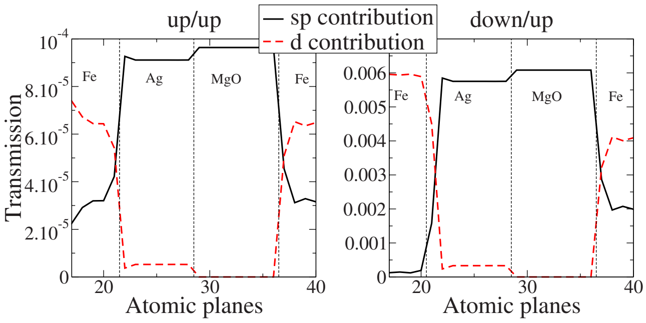

FIG. 7. (Color online) Orbital decomposition of the single conductance channel near the Γ point $k_x = k_y = 0.05$.

The single-orbital model thus demonstrates that large-amplitude oscillations of $\Gamma^{\uparrow\uparrow}$ and $\Gamma^{\downarrow\uparrow}$ and their relative phase shift can be explained by resonant enhancement of these two conductances caused by a potential step created by the Ag interlayer. By examining the conductance of an Fe/Ag bilayer, we have confirmed directly that Ag acts as a potential step both for majority-and minority-spin electrons.

Finally, we need to address the effect of disorder due to interfacial roughness on the resonant enhancement of the TMR. To study disorder, we have performed lateral supercell calculations of the TMR from Eq. (1) for a junction with an intermixing of Fe and Ag atoms at the Fe/Ag interface. As discussed in Ref. 14, lateral supercell calculations for MgO-based junctions are numerically very demanding since a very small imaginary part to the energy, of the order of 10^{-12} Ry, needs to be combined with a very fine mesh of some $10^4 \boldsymbol{k}_{\|}$ points in the irreducible segment of the 2D Brillouin zone to achieve convergence. We have, therefore, used the method in Ref. 14 where the surface Green's functions are first determined using the ordinary nonsupercell basis and only in the last step of "depositing" the mixed layer and connecting the left and right surfaces across the cleavage plane via Eq. (2), does one convert to the supercell basis. This method renders the calculation of the TMR for a disordered junction feasible. In Fig. 8 we show the TMR as a function of Ag thickness both for perfect Fe/Ag interface and for the configuration average over 20 randomly disordered interfaces with 20% intermixing of Fe and Ag atoms. The thickness of the MgO

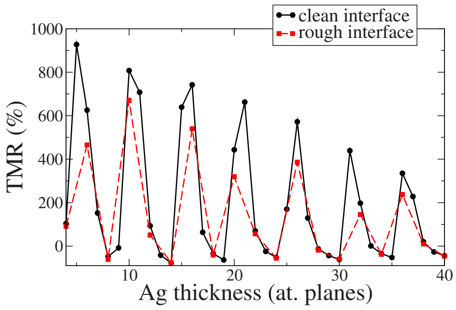

FIG. 8. (Color online) Dependence of the TMR ratio on Ag thickness for a disordered (broken line) and perfectly ordered (continuous line) Fe/Ag/MgO/Fe junction.

barrier in Fig. 8 is eight atomic planes and the size of the supercell used was 8 × 8. It can be seen that the effect of disorder is quite weak, only the amplitude of TMR oscillations is somewhat reduced. We recall that the effect of disorder of the same magnitude on the TMR of Fe/MgO/Fe(001) junction without any Ag interlayer is drastic. In fact, the calculated TMR for Fe/MgO/Fe(001) junction with 20% interfacial intermixing and eight atomic planes of MgO is reduced by a factor of 5 from its value for a perfect junction.[14] Our lateral supercell modeling of interfacial roughness thus indicates that, rather surprisingly, the Fe/Ag/MgO/Fe(001) junction is much more robust against disorder that the Fe/MgO/Fe(001) junction without any interlayer.

IV. CONCLUSIONS

Using the Kubo-Landauer formula and fully realistic tight-binding bands fitted to an *ab initio* band structure, we have investigated the effect of a single Ag interlayer on the tunneling magnetoresistance of an Fe/Ag/MgO/Fe(001) tunneling junction. We find that the TMR ratio of such a junction oscillates as a function of the silver layer thickness between positive values in excess of 2000% and negative values of the order of −100%. The large positive TMR and changes in its sign are due to resonant enhancement of the tunneling conductance $\Gamma^{\uparrow\uparrow}$ of majority-spin carriers in the ferromagnetic configuration and of the conductance $\Gamma^{\downarrow\uparrow}$ of carriers tunneling in the antiferromagnetic configuration from the minority-spin channel in the left Fe electrode (next to the Ag layer) to the majority-spin channel in the right Fe electrode. This mechanism resulting in a very large TMR is quite different from the mechanism that causes large TMR in the standard Fe/MgO/Fe junction without any interlayers. The TMR of an Fe/MgO/Fe junction without an interlayer is large because the conductance at the Γ point in the ferromagnetic configuration is high but the conductance is very low in the antiferromagnetic configuration. This is because tunneling at the Γ point is forbidden in the antiferromagnetic configuration.[1,2] In the case of an Fe/Ag/MgO/Fe(001) junction, both conductances in the ferromagnetic and antiferromagnetic configurations are comparable. A very high positive TMR and oscillations of its sign occur because these conductances oscillate as a function of Ag thickness with comparable amplitudes but with a large phase shift which makes them oscillate almost in antiphase. It follows that by choosing the appropriate Ag interlayer thickness one can tune the magnitude and even the sign of the TMR. It should be noted that this mechanism is also different from resonant tunneling in a double-barrier magnetic junction[3–5] or in a junction with two symmetric nonmagnetic interlayers.[6] In those cases tunneling in only one magnetic configuration of the junction is resonantly enhanced but it remains unenhanced in the other configuration.

Using the lateral supercell method we have also investigated the effect of interfacial roughness on the resonant tunneling in an Fe/Ag/MgO/Fe(001) junction. We find that, in contrast to the simple Fe/MgO/Fe(001) junction whose TMR is reduced drastically by disorder,[14] the Fe/Ag/MgO/Fe(001) junction with silver interlayer is much more robust against disorder. In fact, 20% intermixing at the Fe/Ag interface leads only to a small reduction in the amplitude of TMR oscillations. It is easy to understand why disorder has different effects on the junctions without and with an Ag interlayer. As already discussed, the TMR of a junction without an interlayer is so large because tunneling at the Γ point in the antiferromagnetic configuration is forbidden.[1,2] Disorder opens up the conductance channel at the Γ point in the antiferromagnetic configuration and the TMR thus drops rapidly and saturates with MgO thickness.[14] The situation for the junction with an Ag interlayer is quite different since both the ferromagnetic and antiferromagnetic conductances in the vicinity of the Γ point are already high due to resonant enhancement caused by the Ag interlayer. Large TMR and its change in sign are due to a phase shift between the oscillations of the conductances $\Gamma^{\uparrow\uparrow}$ in the ferromagnetic and $\Gamma^{\downarrow\uparrow}$ in the antiferromagnetic configurations. Since these oscillations at the Γ point have a long period of 5.3 atomic planes determined by the spanning vector of the Ag Fermi-surface belly, interfacial disorder on the scale of an interatomic distance has only a small effect on them.

Finally, we would like to mention that the interlayer resonant tunneling mechanism that leads to a negative TMR is analogous to that which may occur spontaneously as a result of oxidation of Fe at a single MgO/Fe interface.[15] The negative TMR in this case is due to the effect of an interfacial state. However, for this effect to be observable a near perfect oxide layer would have to be formed at the interface. The advantage of using nonmagnetic metallic interlayers is that they can be quite thick and hence need not be so perfect. Moreover, by choosing specific elements such as Ag, Au, or Cu, and also the interlayer thickness there is a potential for tuning the magnitude and even the sign of the TMR.

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