Oscillations with Co and Cu thickness of the current-perpendicular-to-plane giant magnetoresistance of a Co/Cu/Co(001) trilayer

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The results of a rigorous quantum calculation of the current-perpendicular-to-plane giant magnetoresistance (CPP GMR) of a Co/Cu/Co(001) trilayer without impurity scattering are reported. The conductances per spin in the ferromagnetic (FM) and antiferromagnetic (AF) configurations of the magnetic layers are computed from the Kubo formula. The electronic structure of the Cu and Co layers is described by fully realistic s,p,d tight-binding bands fitted to *ab initio* band structures of Cu and ferromagnetic fcc Co. Depending on Co thickness, the CPP GMR ratio can be as high as 90%. The whole calculated effect is due solely to quantum reflections of electrons from perfectly flat Co/Cu interfaces. The CPP GMR ratio is found to oscillate both with Co and Cu thickness, the respective oscillation amplitudes being 12 and 6 % of the average GMR. The resistances in each spin channel per unit cross-sectional area of the trilayer range from 3 to 7 fΩ and oscillate with an amplitude $\sim$ 0.5 fΩ. An analytic asymptotic formula for resistance oscillations originating from the Cu Fermi surface is applied to analyze the numerical results. It is found that the resistance oscillations for majority electrons in the FM configuration have periods dominated by the extremal radii of the Cu Fermi surface. These are the same periods as observed in the oscillatory exchange coupling. However, the amplitude of resistance oscillations with the Fermi-surface periods is negligibly small for the minority electrons in the FM configuration and for electrons of either spin orientation in the AF configuration. The resistance oscillations of these electrons are dominated instead by periods determined by cutoffs of the conductance due to a mismatch between the Co and Cu bands across the Co/Cu interfaces. [S0163-1829(97)05121-7]

I. INTRODUCTION

Since the discovery of the giant magnetoresistance effect[1] (GMR) and oscillatory exchange coupling[2] the transport and magnetic properties of magnetic multilayers have attracted much attention. The conventional explanation of the GMR effect is based on spin-dependent scattering of electrons from magnetic impurities located at the ferromagnet/spacer interfaces (interfacial roughness). However, a fully quantitative theory of the GMR effect is still lacking. This is largely due to the fact that, in the most common current-in-plane geometry, the dimensions of the sample in the direction of the current are always macroscopic. One is, therefore, in the diffusive regime, which means that a fully predictive theory must treat interfacial roughness realistically. It must also be based on an *ab initio* band structure and the transport problem should be treated quantum mechanically. None of the existing theories satisfies all these requirements.

Realistic modeling of interfacial roughness combined with a rigorous quantum evaluation of the GMR was made by Asano *et al.*[3] but only for a single-orbital tight-binding band and very small samples. Nevertheless, the results of their computer modeling of GMR are very interesting since they show that there is a qualitative difference between the current-in-plane (CIP) and current-perpendicular-to-plane (CPP) geometries. Asano *et al.*[3] found that spin-dependent scattering from interfacial roughness is essential for the CIP but is far less important in the CPP geometry. In fact, they showed that the CPP GMR is determined by scattering from potential steps at the interfaces between the magnetic and nonmagnetic layers and has its largest value when the interfaces are perfectly flat. Scattering from perfectly flat interfaces is, of course, also spin dependent because up- and down-spin electrons see different exchange potentials in the ferromagnetic layers.

If one accepts that interfacial roughness is relatively unimportant in the CPP geometry and assumes that the total thickness of the sample is smaller than the mean free path for impurity scattering, which can be easily satisfied experimentally for a trilayer, a fully realistic calculation of the CPP GMR becomes feasible. One then has a well-defined system for which a quantitative comparison between theory and experiment is meaningful. A fundamental question that arises is whether scattering from perfectly flat interfaces in such an ideal trilayer leads to a measurable CPP GMR. To answer this question, one has to calculate the absolute values of the total resistances of a specific trilayer in each of its magnetic configurations rigorously, i.e., without any adjustable parameters. We report here the results of such a calculation for a Co/Cu/Co(001) trilayer sandwiched between two semi-infinite Cu leads. The calculation is based on an exact numerical evaluation of the real-space Kubo formula using tight-binding parametrization with s,p,d bands and hopping to first and second neighbors of an *ab initio* band structure of Cu and fcc ferromagnetic Co. Our calculations show that the CPP GMR without impurity scattering can be as high as 90% and the total resistance in each spin channel is large enough to be measurable.

We showed recently[4] using a single-orbital tight-binding model that, in the CPP geometry in which scattering from flat interfaces dominates the GMR, quantum interference effects lead necessarily to oscillations of the CPP GMR with the spacer and ferromagnet thickness. The calculations re-

ported here confirm that such quantum oscillations of the CPP GMR occur in Co/Cu/Co(001) and have relatively large amplitudes. In the cases of a single-orbital tight-binding and parabolic bands, we also predicted in Ref. 4 oscillation periods that are not related to the spacer Fermi surface. Here we demonstrate that such periods are also present in Co/Cu/Co(001) trilayer.

II. KUBO FORMULA FOR MULTIORBITAL TIGHT-BINDING HAMILTONIAN IN TERMS OF GREEN'S FUNCTIONS

We calculate the CPP-GMR of a Co/Cu/Co(001) trilayer in the usual two-probe geometry.[5] The trilayer consists of two ferromagnetic fcc Co layers of M atomic planes each separated by N atomic planes of Cu. It is sandwiched between two semi-infinite Cu lead wires assumed to have negligible resistance. Leads with a negligible resistance can be realized experimentally by using a superconducting metal such as Nb,[6] or by making the trilayer in the form of a thin pillar sandwiched between thick leads.[7] Both the trilayer and the lead wires are described by fully realistic s,p,d tight-binding bands with hopping to first- and second-nearest neighbors fitted to *ab initio* band structures of Cu and fcc ferromagnetic Co. A small lattice mismatch between Co and Cu is neglected and the whole layer structure is taken to have the lattice parameter of bulk Cu. We also assume that the local potentials in the Cu and Co layers are frozen, i.e., they do not change in going from the antiferromagnetic (AF) to the ferromagnetic (FM) configuration of the magnetic moments in the Co layers. Finally, we assume an abrupt interface between Co and Cu and calculate the GMR of the structure neglecting any impurity scattering (the sample is assumed to be smaller in all directions than the mean free path).

The GMR ratio is defined in terms of the conductances for up- and down-spin electrons in the ferromagnetic and antiferromagnetic configurations of the magnetic layers by

$$\mathrm{GMR}=(\Gamma^{\uparrow}_{\mathrm{FM}}+\Gamma^{\downarrow}_{\mathrm{FM}}-2\Gamma^{\uparrow,\downarrow}_{\mathrm{AF}})/2\Gamma^{\uparrow,\downarrow}_{\mathrm{AF}}, \tag{1}$$

where $\Gamma^{\sigma}_{\mathrm{FM\,(AF)}}$ is the conductance for a given spin channel σ in the FM (AF) configuration of the magnetic layers. Each of the conductances in Eq. (1) can be calculated using linear-response theory. The starting point of such a calculation is the Kubo formula[8,9] for the frequency-dependent conductance at zero temperature

$$\Gamma(\omega)=\frac{\pi}{\omega}\int dE\sum_{n,m}|\langle n|I|m\rangle|^2\delta(E+\hbar\omega-E_m)\,\delta(E-E_n), \tag{2}$$

where we have suppressed the spin index σ. The quantity I in Eq. (2) is the total current operator and the sum over n,m is over all the energy eigenstates $|n\rangle,|m\rangle$ of the system with energies E_n,E_m such that $E_n<E_F<E_m$, where E_F is the Fermi energy.

It is convenient to express Eq. (2) in terms of one-electron Green's functions. We first require a general expression for the current operator for a multiorbital tight-binding band structure. We start by calculating the rate of change of the total number of particles, $\int_V\rho dV$, in an arbitrary volume V enclosed by a surface S. The particle density operator is $\rho=\Sigma_{i,j}\Sigma_{\alpha,\beta}c^{\dagger}_{i\alpha}c_{j\beta}\phi^{\dagger}_{i\alpha}\phi_{j\beta}$ where i,j label lattice sites contained in the volume V, α,β are orbital indices, and $c^{\dagger}_{i\alpha}$ ($c_{i\alpha}$) is the creation (annihilation) operator of a one-particle state in the atomic orbital α at a site $\boldsymbol{r}_i$. The rate of change, $(\partial/\partial t)\int_V\rho dV$, can be evaluated from the equation of motion for ρ using the tight-binding kinetic energy operator $T=\Sigma_{\alpha,\beta}c^{\dagger}_{i\alpha}c_{j\beta}t_{i\alpha,j\beta}$, where $t_{i\alpha,j\beta}$ is the matrix of hopping integrals. Since the atomic orbitals are localized, we assume the wave functions to be approximately orthogonal over the volume V. The total current across the surface S is then obtained from the equation of continuity $(\partial/\partial t)\int_V\rho dV+I=0$. Taking into account the fact that terms for which both $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$ belong to V give zero contribution to the current, we obtain

$$I=\frac{ie}{\hbar}\sum_{\substack{\boldsymbol{r}_i\in V\\ \boldsymbol{r}_j\notin V}}\sum_{\alpha,\beta}(t_{i\alpha,j\beta}c^{\dagger}_{i\alpha}c_{j\beta}-t_{j\beta,i\alpha}c^{\dagger}_{j\beta}c_{i\alpha}). \tag{3}$$

Equation (3) gives the total current flowing across the surface S enclosing an arbitrary volume V.

We can apply Eqs. (2) and (3) to any multilayer sample. We assume the sample to be separated into two parts by an imaginary plane passed between any two neighboring atomic planes. For convenience, we refer to the left and right parts of the sample as left and right overlayers on the ideal leads. It should be noted, however, that no real physical separation takes place at this stage. The volume V is then taken to be the volume enclosing, say, the left overlayer. Our aim is to determine the current flowing from the left to the right overlayer. Taking into account the layer geometry of the problem, we write $\boldsymbol{r}_i=(\boldsymbol{R}_{\parallel},\ell),\boldsymbol{r}_j=(\boldsymbol{R}'_{\parallel},\ell')$, where $\boldsymbol{R}_{\parallel},\boldsymbol{R}'_{\parallel}$ are the two-dimensional position vectors in the plane of the layers and ℓ,ℓ' are site indices in the direction perpendicular to the layers. Because of the current conservation, the choice of the atomic planes between which the imaginary ''cleavage'' plane is passed is arbitrary. For simplicity, we denote by $\ell=0$ the atomic plane on the left of the cleavage plane and by $\ell'=1$ that on the right of the cleavage plane. The current across the cleavage plane is then given by

$$\begin{aligned}I&=\frac{ie}{\hbar}\sum_{\boldsymbol{R}_{\parallel}}\sum_{\boldsymbol{R}'_{\parallel}}\sum_{\alpha,\beta}(t_{0\alpha,1\beta}c^{\dagger}_{0\alpha}c_{1\beta}-t_{1\beta,0\alpha}c^{\dagger}_{1\beta}c_{0\alpha})\\&=\frac{ie}{\hbar}\sum_{\boldsymbol{k}_{\parallel}}\sum_{\alpha,\beta}[t_{0\alpha,1\beta}(\boldsymbol{k}_{\parallel})c^{\dagger}_{0\alpha}c_{1\beta}-t_{1\beta,0\alpha}(\boldsymbol{k}_{\parallel})c^{\dagger}_{1\beta}c_{0\alpha}].\end{aligned} \tag{4}$$

We have transformed in Eq. (4) to a mixed Bloch-Wannier representation using $|\boldsymbol{R}_{\parallel}\rangle=N_{\parallel}^{-1/2}\Sigma_{\boldsymbol{k}_{\parallel}}\exp(-i\boldsymbol{k}_{\parallel}\cdot\boldsymbol{R}_{\parallel})|\boldsymbol{k}_{\parallel}\rangle$, where $\boldsymbol{k}_{\parallel}$ is the wave vector and $N_{\parallel}$ is the number of atoms in the direction parallel to the layers. The sum is over all $\boldsymbol{k}_{\parallel}$ in the two-dimensional Brillouin zone.

To calculate the frequency-dependent conductance, we first extend the sum over n,m in Eq. (2) to a sum over a complete set of eigenstates using the identity

$$\sum_{\substack{n,m \\ E_n<E_F<E_m}} |\langle n|I|m\rangle|^2 = \sum_{\{|n\rangle\},\{|m\rangle\}} |\langle n|I|m\rangle|^2 \lim_{T\to 0^+} f(E_n)[1-f(E_m)], \tag{5}$$

where the curly brackets indicate complete sets of eigenstates and $f(E)$ is the Fermi function. Using Eq. (4) for the current operator and inserting complete sets of one-electron states in the matrix elements in Eq. (5), we can rewrite Eq. (2) in terms of the advanced and retarded one-electron Green's functions, $G^{\pm}_{i\alpha,j\beta}(\boldsymbol{k}_\parallel)=\langle i,\boldsymbol{k}_\parallel,\alpha|(E-H\pm i\epsilon)^{-1}|j,\boldsymbol{k}_\parallel,\beta\rangle$, where H is the Hamiltonian operator and ϵ is a small positive number. This is achieved by noting that

$$\tilde{G}_{i\alpha,j\beta}(\boldsymbol{k}_\parallel)=\frac{1}{2i}[G^{-}_{i\alpha,j\beta}-G^{+}_{i\alpha,j\beta}] = \pi\sum_{\mathcal{M}} \langle\mathcal{A}|n\rangle\langle n|\mathcal{B}\rangle\,\delta(E-E_n), \tag{6}$$

where gothic letters have been used to label one-electron states of the type $|i,\boldsymbol{k}_\parallel,\alpha\rangle$.

The total conductance then reduces to

$$\begin{aligned}\Gamma(\omega)=\frac{e^2}{\pi\hbar^2\omega}\sum_{\boldsymbol{k}_\parallel}\lim_{T\to 0^+}\int dE f(E)[1-f(E+\hbar\omega)] \\ \times\sum_{\alpha,\beta,\mu,\nu}\{t_{1\beta,0\alpha}t_{0\mu,1\nu}\tilde{G}_{1\nu,1\beta}(E)\tilde{G}_{0\alpha,0\mu}(E+\hbar\omega) \\ +t_{0\alpha,1\beta}t_{1\nu,0\mu}\tilde{G}_{0\mu,0\alpha}(E)\tilde{G}_{1\beta,1\nu}(E+\hbar\omega) \\ -t_{0\alpha,1\beta}t_{0\mu,1\nu}\tilde{G}_{1\nu,0\alpha}(E)\tilde{G}_{1\beta,0\mu}(E+\hbar\omega) \\ -t_{1\beta,0\alpha}t_{1\nu,0\mu}\tilde{G}_{0\mu,1\beta}(E)\tilde{G}_{0\alpha,1\nu}(E+\hbar\omega)\}.\end{aligned}$$

The dc conductance is obtained in the limit $\omega\to 0^+$. Restoring the spin index σ and making some trivial rearrangements, we arrive at the following expression for the conductance in the spin channel σ:

$$\Gamma^\sigma=\frac{e^2}{h}\sum_{\boldsymbol{k}_\parallel}\Gamma^\sigma(\boldsymbol{k}_\parallel) = \frac{4e^2}{h}\sum_{\boldsymbol{k}_\parallel}\mathrm{ReTr}(\tilde{G}^\sigma_{00}t^\sigma_{01}\tilde{G}^\sigma_{11}t^\sigma_{10}-t^\sigma_{01}\tilde{G}^\sigma_{10}t^\sigma_{01}\tilde{G}^\sigma_{10}). \tag{7}$$

Here, the trace is over all orbital indices that are contained implicitly in the layer indices 0 and 1, $t^\sigma_{01}(\boldsymbol{k}_\parallel)$ is the tight-binding hopping matrix between the layers 0,1, and all the Green's functions are evaluated at E_F. It can be seen that the total conductance is the sum of partial conductances $\Gamma^\sigma(\boldsymbol{k}_\parallel)$ measured in units of the quantum conductance e^2/h. Equation (7) is a multiband generalization of the result obtained by Lee and Fisher[8] for a single-orbital tight-binding model. It is exact within the linear-response theory.

For simplicity, we derived Eq. (7) assuming hopping to nearest neighbors only. However, Eq. (7) holds also in the case of hopping to more distant neighbors provided atomic planes are replaced by principal layers.[10] In the case of hopping to second neighbors considered here, each principal layer contains two atomic (001) planes and all the Green's functions and hopping matrices in Eq. (7) are, therefore, 18×18 matrices. With this qualification, Eq. (7) can be readily applied to a Co/Cu/Co trilayer with hopping to second-nearest neighbors.

III. TRANSMISSION COEFFICIENTS

To check the numerical accuracy of the evaluation of the conductance from the Kubo formula, we first use Eq. (7) to calculate the energy dependence of the ballistic conductance of pure Cu and pure Co. The input in Eq. (7) are the matrix elements of the tight-binding Green's function for bulk Cu and Co. We determine the bulk Green's functions in two stages. In the first stage, we compute the surface matrix elements of the Green's function for semi-infinite Cu (Co) crystals occupying the half-space to the left of the principal plane 0 and the half-space to the right of the plane 1. The two semi-infinite crystals are now assumed to be physically separated and the cleavage plane between the planes 0 and 1 is, therefore, real. The corresponding surface matrix elements are denoted by g_{00} and g_{11}. In the second stage, electron hopping between the planes 0 and 1 is turned on, i.e., the two semi-infinite crystals are reconnected and the required Green's-function elements G^σ_{00}, G^σ_{11}, and G^σ_{10} for the connected bulk crystal are obtained from g_{00} and g_{11} using the Dyson equation. This might seem a rather indirect method for computing the bulk Green's function but we adopt it here because it can be very easily generalized to calculate the local Green's functions in an arbitrary layer structure.

The only remaining problem is, therefore, the calculation of the surface Green's functions of the left and right semi-infinite crystals. In our previous calculations[11] of the exchange coupling in Co/Cu(001), we used an iterative decimation technique.[12] In this method, the surface Green's function is approximated by that at the surface of a thick stack of atomic planes. However, to obtain a truly surface Green's function, it is necessary to add in the decimation method a small imaginary part ϵ to the energy to disrupt quantum interference effects between the two surfaces of the slab. When ϵ is small the convergence of the decimation method becomes poor. This is not a problem in total-energy calculations since one integrates over a contour in the complex energy plane. However, there is no energy integral in the Kubo formula (transport takes place at the Fermi surface) and ϵ has to be very small in order not to introduce a spurious resistance due to finite lifetime effects. We have, therefore, used an entirely noniterative technique for generating the surface Green's function[13] in which the convergence problem does not arise. A value $\epsilon=10^{-8}$ Ry, which was used in all our calculations, is so small that it has no effect on the conductance.

The energy dependence of the ballistic conductance of bulk Cu and Co determined from the Kubo formula is shown in Fig. 1. Note that the conductances for the majority and minority-spin channels in ferromagnetic Co have been shifted so that the Fermi energy of Co coincides with that of bulk Cu.

To calculate the conductance of a perfectly periodic infinite sample, it is not really necessary to evaluate the one-electron Green's functions required in Eq. (7). It was noted by Schep *et al.*[14] that, in this case, it is much easier to evalu-

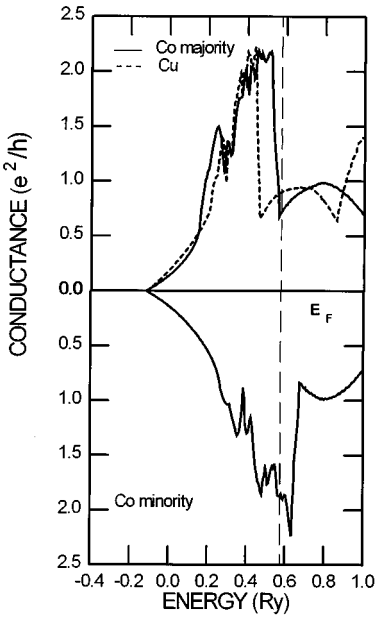

FIG. 1. Ballistic conductance per atom of bulk Cu and Co determined from the Kubo formula. The conductances for the majority and minority spin channels in Co have been shifted so that the Fermi energy of Co coincides with that of bulk Cu.

ate the conductance from the Landauer formula[15]

$$\Gamma^{\sigma}=\frac{e^2}{h}\sum_{\boldsymbol{k}_{\parallel}} T^{\sigma}(\boldsymbol{k}_{\parallel}), \tag{8}$$

where $T^{\sigma}(\boldsymbol{k}_{\parallel})$ is the transmission coefficient in the channel $(\boldsymbol{k}_{\parallel},\sigma)$. Given that the transmission probability of each propagating (band) state at a given energy is equal to unity, counting the number of such states yields the conductance at that energy.[14] Since it was shown by Fisher and Lee[16] that the Kubo formula (7) is equivalent to the Landauer formula (8), we have used this alternative method as an independent check on the accuracy of our evaluation of the conductance from the Kubo formula (7). The conductance of a bulk Cu (Co) crystal obtained from the Landauer formula (8) is identical with the results shown in Fig. 1 that were calculated from the Kubo formula (7). Our results also agree with the calculations of the ballistic conductance of Cu (Co) made by Tsymbal[17] using the Landauer formula (counting argument).

Note that the actual ballistic conductance per unit area of bulk Cu at the Fermi energy is $0.54\times10^{15}\Omega^{-1}\ \mathrm{m}^{-2}$, which is in excellent agreement with the result of Bauer.[5] The conductances (per unit area) at E_F for the majority- and minority-spin channels in ferromagnetic fcc Co are $0.43\times10^{15}\Omega^{-1}\ \mathrm{m}^{-2}$ and $1.1\times10^{15}\Omega^{-1}\ \mathrm{m}^{-2}$, respectively. It follows that the conductance of Co in the majority spin channel is close to that of pure Cu. It should be also noted that a slight shift in the position of the Fermi energy (e.g., due to temperature or lattice relaxation effects) could lead to a dramatic change in the conductance of Co in the majority-spin channel.

Having tested the accuracy of our approach based on the Kubo formula for bulk Cu and Co, we now apply the method to a Co/Cu(001) trilayer. In Ref. 4 we predicted for a single-orbital tight-binding model that quantum interference effects should lead to oscillations of the CPP GMR with nonmagnetic spacer layer thickness. In contrast to the oscillatory exchange coupling in magnetic multilayers, the CPP GMR was shown to oscillate not only with the expected Fermi-surface (FS) periods but also with additional periods determined by the potential steps between the magnetic and nonmagnetic layers. The physical origin of the oscillation periods was explained in Ref. 4 but the single-orbital tight-binding or parabolic band models used in Ref. 4 cannot predict the correct periods and amplitudes of CPP GMR oscillations in real systems. We now investigate these quantum oscillations in a Co/Cu/Co(001) trilayer using fully realistic s,p,d tight-binding bands.

The conductance in a channel $(\boldsymbol{k}_{\parallel},\sigma)$ vanishes in the CPP geometry when the electrons of spin σ at E_F with that particular value of $\boldsymbol{k}_{\parallel}$ become totally reflected from either the left or right ferromagnet. Such cutoffs in the transmission probability of electrons at E_F were shown in Ref. 4 to lead to additional oscillation periods. It is, therefore, interesting first to examine the behavior of the transmission coefficients in the $\boldsymbol{k}_{\parallel}$ plane for up- and down-spin electrons in the FM and AF configurations of the magnetic layers.

The transmission coefficients $\Gamma^{\sigma}(\boldsymbol{k}_{\parallel})$ for the Co/Cu/Co(001) trilayer are calculated from Eq. (7). To evaluate the matrix elements of the advanced and retarded Green's functions required in Eq. (7), we generalize the method that has been applied to calculate the conductance of bulk Cu (Co). We pass a real cleavage plane between the principal planes 0 and 1 in the Cu spacer which separates the trilayer into independent left and right overlayers. The left overlayer consists of the semi-infinite Cu lead wire, the M atomic planes of Co and one principal plane (two atomic planes) of Cu. The right overlayer contains the right semi-infinite Cu lead, M atomic planes of Co and $N-2$ atomic planes of Cu. The surface Green's functions g_{00},g_{11} for the isolated left and right overlayers are calculated recursively from the surface Green's functions of the semi-infinite leads by the method of adlayers.[18] The calculation of the surface Green's functions for the semi-infinite Cu leads has already been described. The final step is to reconnect the left and right overlayers using the Dyson equation. It is easy to show that the matrix elements of the Green's functions for the connected sample are given by $G_{00}=(1-g_{00}t_{01}g_{11}t_{10})^{-1}g_{00}$, $G_{11}=(1-g_{11}t_{10}g_{00}t_{01})^{-1}g_{11}$ and $G_{10}=g_{11}t_{10}(1-g_{00}t_{01}g_{11}t_{10})^{-1}g_{00}$. We stress that the method of adlayers involves no approximations and, therefore, all the local Green's functions are obtained with machine accuracy.

Figures 2(a) and 2(b) display the $\boldsymbol{k}_{\parallel}$ dependence of the partial conductances (transmission coefficients) for up- and down-spin electrons in the FM configuration of the magnetic layers. The results shown in Fig. 2 are for a system consisting of six atomic planes of Cu sandwiched between thick (semi-infinite) Co layers. Figure 2(c) shows the transmission coefficients for electrons of either spin orientation in the antiferromagnetic configuration. The values of $\boldsymbol{k}_{\parallel}$ for which the transmission goes to zero lie on a boundary along which cutoffs occur and from which different periods may arise. It can be seen from Fig. 2(a) that the transmission coefficient is close to unity over a large region of $\boldsymbol{k}_{\parallel}$ space for the up-spin electrons in the FM configuration. This is due to the fact that

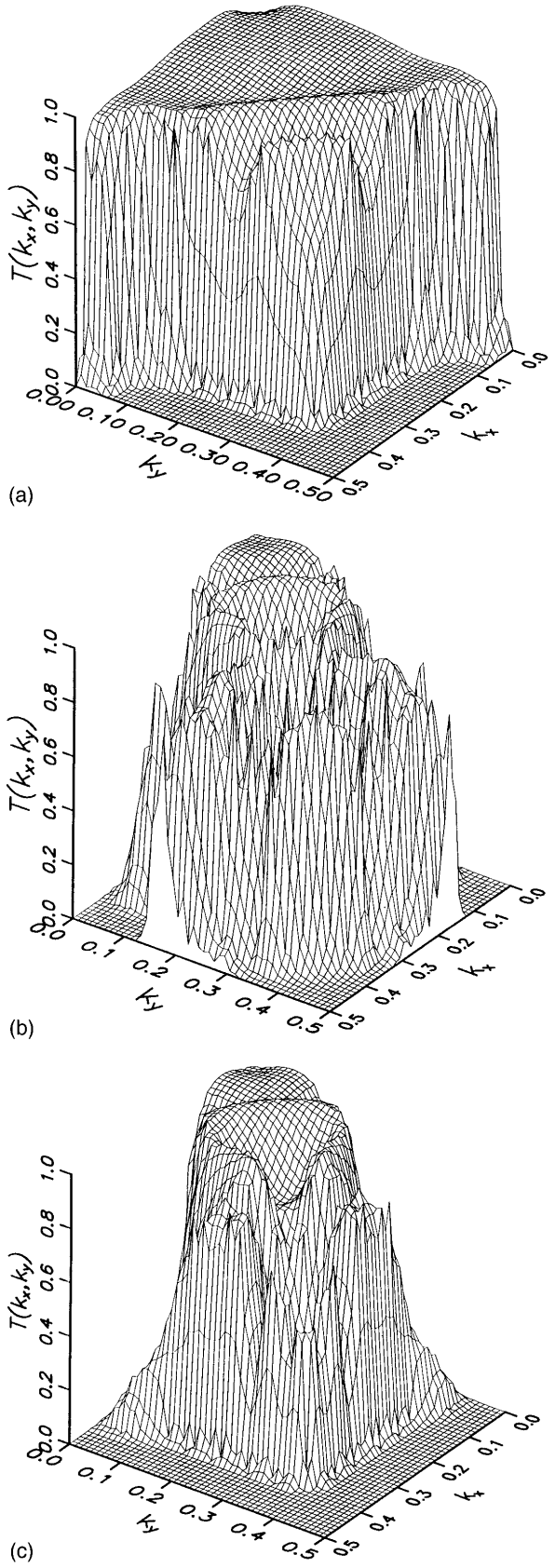

FIG. 2. Partial conductances (transmission coefficients) of a Cu layer sandwiched between two semi-infinite Co layers as a function of (k_x, k_y) (in units of π/d) for (a) up- and (b) down-spin electrons in the FM configuration and (c) for electrons of either spin in the AF configuration.

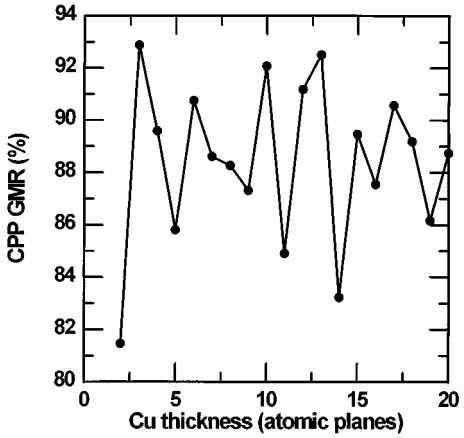

FIG. 3. CPP GMR ratio versus Cu thickness for a trilayer with seven atomic planes of Co in each magnetic layer.

the band structures of Cu and of majority-spin Co are very well matched and, therefore, electrons propagate across the whole structure with virtually no scattering and make a large contribution to the conductance. For the minority electrons, there is a large band mismatch between Co and Cu bands which means that the transmission is poor. Similarly, transmission of electrons of either spin orientation is poor in the antiferromagnetic configuration. We shall see later that this contrast between the minority electrons in the FM configuration and electrons of either spin configuration in the AF configuration leads to a large value of the CPP GMR.

IV. CPP RESISTANCES AND GMR

Using the results of Sec. III, it is easy to calculate the CPP GMR by simply summing the partial conductances Γ^{σ} for each spin channel over all $\boldsymbol{k}_{\parallel}$ in the two-dimensional (2D) Brillouin zone (BZ). The nonoscillatory component of the GMR ratio is obtained relatively easily but to study GMR oscillations requires a far greater accuracy in the evaluation of the BZ sum. It is, therefore, very important to ensure that convergence has been achieved in the summation over $\boldsymbol{k}_{\parallel}$. For a trilayer having a thickness of about 10 nm ($\sim$ 50 atomic planes), we have used 9×10^4 $\boldsymbol{k}_{\parallel}$ points in the 2D Brillouin zone. The results differ from those obtained with $4\times10^4\boldsymbol{k}_{\parallel}$ points by less than 0.5% and are, therefore, deemed to be converged.

Figure 3 shows the dependence of the CPP-GMR ratio on the Cu spacer layer thickness for a trilayer with seven atomic planes of Co in each magnetic layer. A GMR ratio of about 90% is obtained. Since we neglect impurity scattering, this large ratio is due entirely to reflections of electrons from perfectly flat Co/Cu interfaces. Superimposed on the constant value of the CPP GMR are oscillations whose amplitudes are about 6% of the total GMR. These oscillations are due to quantum interference effects and have, therefore, the same origin as the oscillatory exchange coupling.[4] The exchange coupling has been shown to oscillate also as a function of the ferromagnetic layer thickness.[19–22] Therefore, we expect the CPP GMR to oscillate also with Co layer thickness. This is indeed the case, and the cobalt-thickness dependence of the GMR ratio at the first antiferromagnetic peak ($\sim$ six atomic planes of Cu) is displayed in Fig. 4. Oscilla-

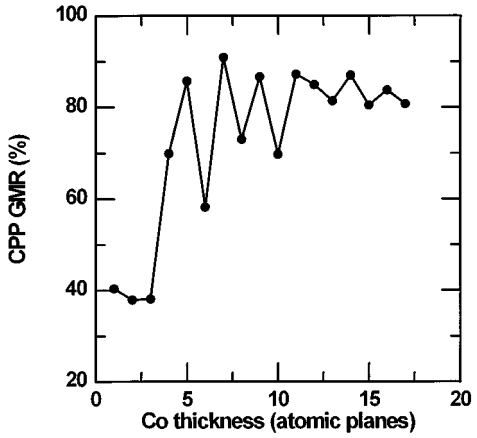

FIG. 4. Cobalt-thickness dependence of the CPP GMR ratio of a Co/Cu/Co trilayer at the first antiferromagnetic peak (six atomic planes) of Cu.

tions having an amplitude ~ 12% of the total GMR of about 80% are obtained.

To clarify the origin of the GMR oscillations, the individual resistances for up- and down-spin electrons in the FM and AF configurations are shown in Fig. 5. The lowest resistance and smallest oscillation amplitude occur for the up-spin electrons in the FM configuration. This is easily understood in terms of the band structures of bulk Co and Cu. The bands of Co and Cu are very well matched for the majority electrons and, therefore, there is virtually no interfacial scattering. This leads to a low resistance and weak quantum interference effects. For the minority electrons, there are band offsets between Co and Cu and, therefore, interfacial scattering is important. It leads to a larger value of the resistance for the down-spin electrons. For the same reason, the resistance in the AF configuration is also high for electrons of either spin orientation. Quantum interference effects are more pronounced and are reflected in large-amplitude oscillations of the resistance in these two cases. For the up-spin electrons in the FM configuration, we find a nonoscillatory component $R_{\mathrm{FM}}^{\uparrow}=(2.849/A)\ \mathrm{f}\Omega$ with superimposed oscillations of amplitude $\sim(0.012/A)\ \mathrm{f}\Omega$, where A is the cross-sectional area of the trilayer. The resistance for the down-spin electrons is about twice as large $(5.687/A)\ \mathrm{f}\Omega$ and the oscillations have an amplitude of about $(0.585/A)\ \mathrm{f}\Omega$. In the antiferromagnetic configuration, $R_{\mathrm{AF}}^{\uparrow,\downarrow}=(6.858/A)\ \mathrm{f}\Omega$ and the oscillation amplitude is $\sim(0.502/A)\ \mathrm{f}\Omega$. In samples of transverse cross section 1 mm^2, these resistances are of the order of $10^{-9}\Omega$. Resistances as low as $10^{-12}\Omega$ can accurately be measured using a superconducting quantum interference device (SQUID)-based measuring technique.[23] The resistances mentioned above should, therefore, be observable. The oscillations themselves would become accessible to experiment in samples of transverse cross section 0.1 mm^2.

Finally we analyze in more detail the CPP GMR oscillations as a function of Cu thickness. In order to determine the origin of the oscillation periods, we again examine the individual resistances in each spin channel in the FM and AF configurations. For simplicity, we only discuss the resistance oscillations for a Cu spacer layer sandwiched between two semi-infinite Co layers. The total GMR in this case is much

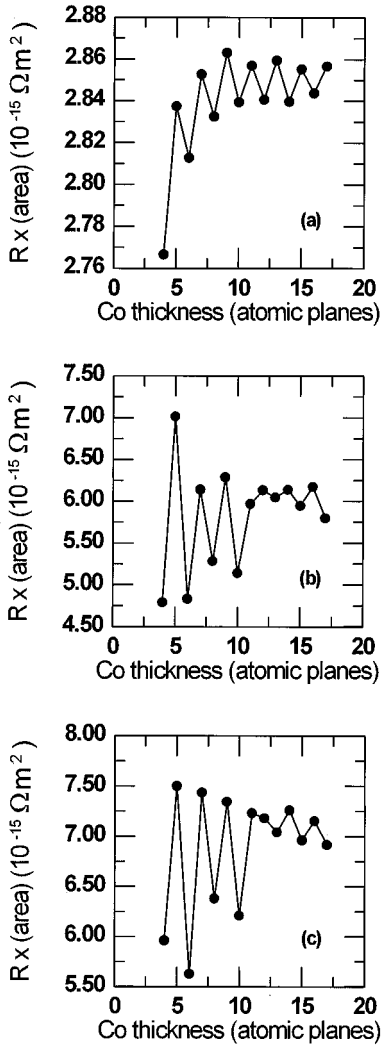

FIG. 5. Resistances for (a) up- and (b) down-spin electrons in the FM configuration and (c) for electrons of either spin in the AF configuration as a function of Co thickness.

smaller (~37%) but the oscillation periods and amplitudes are unaffected by the thickness of the Co layers as long as it is larger than about 5 or 6 atomic planes.

As discussed in Ref. 4, we expect two types of oscillation of the CPP GMR as a function of Cu thickness. The first type originates from extrema of the Cu Fermi surface. The second type is due to cutoffs of the transmission coefficients which occur when the electrons become confined and, therefore, cease to contribute to the conductance. In general, the two types of oscillation are always present but whether any particular oscillation period is actually seen depends on its amplitude. The amplitude and decay with spacer thickness N of any given oscillation can be determined from the asymptotic expansions of the resistance (conductance) valid for large spacer thickness N. We derived in Ref. 4 such asymptotic expansions for both types of oscillation but the asymptotic expansion about a cutoff point (which is much more difficult) was obtained only in the simplest case of a parabolic band. It is, therefore, not directly applicable to a more realistic band structure. An extension of this work to a multi-orbital tight-binding model is currently under way and will be described elsewhere. On the other hand, the conductance

oscillations arising from the points (k_x^0, k_y^0) in the $\boldsymbol{k}_\parallel$ plane at which the perpendicular wave vector $k_\perp$ is stationary can be obtained for an arbitrary band structure. The derivation of an asymptotic formula in this case was described in Ref. 4 and we quote here merely the results. The oscillatory contribution to the conductance in a spin channel σ at a stationary point $\boldsymbol{k}_\parallel{}^0$ is given by

$$\Gamma_{\rm osc}^{\sigma}=\frac{1}{R_{\rm osc}^{\sigma}}=\frac{N_\parallel}{4\pi}\mathrm{Re}\sum_{r=1}^{\infty}\tau c_r(\boldsymbol{k}_\parallel{}^0)m^{\star}e^{2irk_\perp^0 dN}/rN. \qquad (9)$$

Here, $c_r(\boldsymbol{k}_\parallel{}^0)$ are the coefficients of a Fourier series expansion of the partial conductance $\Gamma^{\sigma}(\boldsymbol{k}_\parallel)$ given by Eq. (7), $m^{\star}=|[\partial^2(k_\perp d)/\partial(k_x d)^2][\partial^2(k_\perp d)/\partial(k_y d)^2]|^{-1/2}$ is the curvature of the FS at the stationary point $\boldsymbol{k}_\parallel{}^0$, d is the interplanar distance, and $\tau=i$ when both derivatives in $m^{\star}$ are positive, $\tau=-i$ when they are negative, and $\tau=1$ when the two derivatives have opposite signs.

Comparison of the results obtained from Eq. (9) with the results of a full numerical calculation allows us to determine the relative importance of the FS oscillations. We recall that these are the *only* oscillations that contribute to the oscillatory exchange coupling.[11] In this case, as in the theory of the oscillatory exchange coupling, the oscillation periods $\pi/(k_\perp d)$ are obtained from the Cu FS extremal radii in the [001] direction. There are two extremal radii $k_\perp^0 d=2.586$ occurring at $\boldsymbol{k}_\parallel{}^0=(0,0)$ (belly) and $k_\perp^0 d=1.931$ at $\boldsymbol{k}_\parallel{}^0 a=(\pm 2.53,\pm 2.53)$ (necks), where a is the lattice constant of Cu. The factor $\tau=i$ for the belly and $\tau=1$ for the necks. The ''effective masses'' are $m^{\star}=0.708$ and $m^{\star}=0.538$ for the belly and neck contributions, respectively.

The last step required in the evaluation of Eq. (9) is the Fourier analysis of the partial conductances $\Gamma^{\sigma}(\boldsymbol{k}_\parallel{}^0)$. We used two different methods. The first method is a straightforward adaptation of the approach we applied to determine the oscillatory exchange coupling in Co/Cu(001).[11] The partial conductance $\Gamma^{\sigma}(\boldsymbol{k}_\parallel{}^0)$, which is a periodic function of the spacer thickness, was first computed for discrete (physical) values of the Cu thickness $L=Nd$ and then continued analytically to all real L. The computed values of $\Gamma^{\sigma}(\boldsymbol{k}_\parallel{}^0)$ were then shifted to the first period$(-\pi/2k_\perp,\pi/2k_\perp)$ by subtracting from N the appropriate integral number of periods p and Fourier analyzed.

The second method is an extension of the approach proposed by Umerski.[13] It enables us to compute the local Green's functions and, therefore, $\Gamma^{\sigma}(\boldsymbol{k}_\parallel{}^0)$ directly for fractional values of the interplanar distance d. Not only is the Fourier analysis simplified when this technique is used but, much more importantly, the total conductance can also be computed numerically from Eq. (7) for fractional values of d. When the conductance is a superposition of a number of oscillations with different periods, this method offers a unique opportunity to deduce all the periods from the computed continuous $\Gamma^{\sigma}(\boldsymbol{k}_\parallel{}^0)$ curves. This is virtually impossible when values of the conductance are available only for discrete (physical) values of the spacer thickness $L=Nd$, which is the case in any other conventional calculation.

For the majority electrons in the FM configuration, both belly and neck periods contribute to the oscillations of the conductance. The total oscillatory contribution calculated from Eq. (9) is shown in Fig. 6 (dashed curve) together with the numerical results (solid curve). The physical values of the conductance at discrete atomic plane positions are indicated by circles; the solid curve is calculated from Eq. (7) using the method of Umerski[13] discussed above. A constant background has been subtracted from the numerical results to facilitate the comparison. It is clear from Fig. 6 that the asymptotic formula at the stationary points of the Fermi surface leads to conductance oscillations in good overall agreement with the numerical results. Small discrepancies between the two sets of results are most likely due to contributions arising from cutoffs of the partial conductance. Clearly, the main contribution to the oscillatory conductance comes from the extremal radii of the Cu FS.

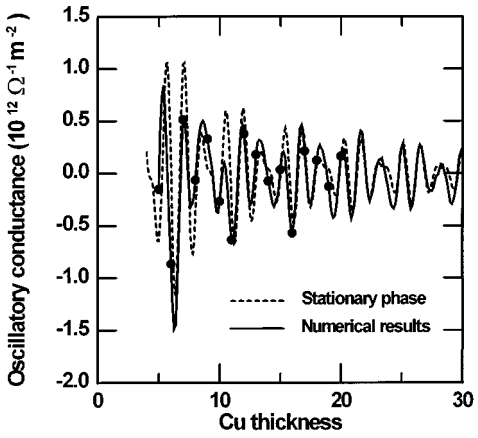

FIG. 6. Oscillatory part of the conductance for up-spin electrons in the FM configuration. Solid curve: numerical results from Eq. (7); dashed curve: stationary phase results from Eq. (9).

In striking contrast are the results for the conductance of the down-spin electrons in the FM configuration and the conductance in the AF configuration. They are displayed in Figs. 7 and 8. In both these cases, the only contribution from the extrema of the FS come from the belly. The electrons with $\boldsymbol{k}_\parallel$ at the neck are confined in the Cu layer and do not contribute to the conductance. The stationary phase results given by the dashed curves in Figs. 7 and 8 are obviously far too

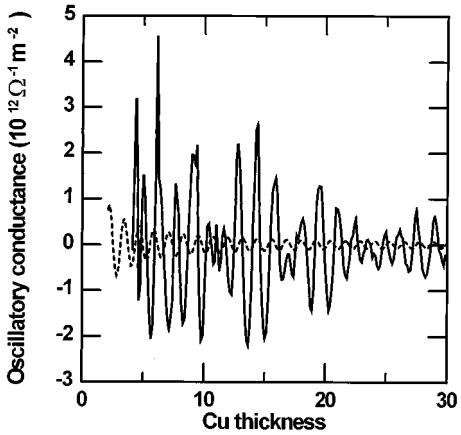

FIG. 7. Oscillatory part of the conductance for down-spin electrons in the FM configuration. Solid curve: numerical results from Eq. (7); dashed curve: stationary phase results from Eq. (9).

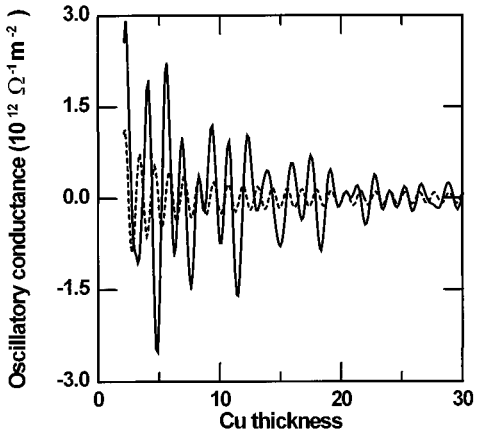

FIG. 8. Oscillatory part of the conductance for up- or down-spin electrons in the AF configuration. Solid curve: numerical results from Eq. (7); dashed curve: stationary phase results from Eq. (9).

small and the oscillations do not have the right period to explain the numerical results. Therefore, we conclude that the conductance oscillations of the minority electrons in the FM configuration and those of electrons of either spin orientation in the AF configuration are totally dominated by the periods predicted in Ref. 4 which are determined by the conductance cutoffs due to band mismatch.

V. CONCLUSIONS

We have investigated comprehensively the perpendicular giant magnetoresistance of a Co/Cu/Co(001) trilayer in the case when a rigorous quantum calculation of the CPP GMR without any adjustable parameters is feasible. Such a calculation is possible provided the dimensions of the trilayer are smaller than the mean free path for scattering from impurities or inhomogeneities of the layer structure other than the interfaces themselves. The CPP GMR was determined by numerical evaluation of the real-space Kubo formula expressed in terms of one-electron Green's functions. This formulation, which is exact in the linear-response theory, is applicable to any layer structure (homogeneous or inhomogeneous) as long as translational invariance in the direction parallel to the layers is preserved.

We find that, depending on the thicknesses of the Co layers, the calculated CPP GMR ratio can be as high as 90%. Since we assume that the mean free path is longer than the sample dimensions, the whole GMR effect is due solely to quantum reflections of electrons from perfectly flat Co/Cu interfaces. In Ref. 4, we predicted that quantum reflections from ferromagnet/spacer interfaces should lead to oscillations of the CPP GMR with the spacer (ferromagnet) thickness. The present calculation, based on a tight-binding parametrization of *ab initio* band structures of Cu and ferromagnetic fcc Co, confirms that the CPP GMR ratio of a Co/Cu/Co(001) trilayer oscillates with Co and Cu thickness and the oscillation amplitudes are large. In fact, we find that the CPP GMR can change by as much as 24% (12%) when the thicknesses of the Co (Cu) layers are varied.

We have also investigated the physical origin of resistance oscillations as a function of Cu thickness. We find that oscillations of the resistance of the majority electrons in the FM configuration are dominated by periods originating from the extremal radii of the Cu Fermi surface in the direction perpendicular to the layers. These are the same periods as observed in the oscillatory exchange coupling. However, the amplitude of resistance oscillations with the Fermi-surface periods is negligibly small for the minority electrons in the FM configuration and for electrons of either spin orientation in the AF configuration. The resistance oscillations of these electrons are dominated instead by periods determined by cutoffs of the conductance due to a mismatch between the Co and Cu bands across the Co/Cu interfaces.[4]

Finally, we discuss briefly the conditions under which the calculated effects should be observable. First of all, the thickness of the Co/Cu/Co trilayer should be smaller than the mean free path for scattering from bulk impurities. This is not difficult to satisfy experimentally. In fact, oscillations in the interlayer exchange coupling, which have been observed in a number of layer structures,[2,19] demonstrate clearly that coherent propagation of electrons from one interface to another takes place in such structures.

The second requirement is that the lead/contact resistance should be much lower than the resistance of the sample. Indeed, this is the physical situation to which the Kubo formula (7) applies. This can be achieved experimentally either by using superconducting leads[6] or by making the trilayer in the form of a thin pillar sandwiched between thick leads.[7] For a pillar of transverse cross section 1 mm^2, the calculated CPP resistances of a Co/Cu/Co(001) trilayer are of the order of $10^{-9}\Omega$. Since resistances as low as $10^{-12}\Omega$ can accurately be measured by a SQUID-based measuring technique,[23] the above resistances should be measurable. The oscillations of CPP GMR we predict would become accessible to experiment in samples of transverse cross section 0.1 mm^2.

In the case of superconducting contacts, one problem that might arise for a trilayer are proximity effects.[24] However, the resistances (CPP GMR) due to scattering from the interfaces are independent of the layer thicknesses as long as they remain smaller than the mean free path (the only inhomogeneity giving rise to a resistance are the interfaces themselves). That means that one could use relatively thick high-purity Cu layers to minimize the proximity effects and hence measure the calculated average CPP GMR. Oscillations of the GMR could not be studied by this method since their amplitudes decay with the spacer layer thickness.

The final point that needs to be addressed is the effect of interfacial roughness (Co/Cu intermixing at the interfaces). Our calculations are for perfectly flat interfaces. The calculations of Asano *et al.*[3] for a single-orbital tight-binding band, which include a realistic modeling of the interfacial roughness, show that the CPP GMR is largest for perfectly flat interfaces. Our results should, therefore, be regarded as an upper theoretical bound on the CPP GMR of a Co/Cu/Co(001) trilayer.

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