Giant-magnetoresistance calculation for {111} Co/Cu/Co spin valves

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We calculate the canting-angle and thickness dependence of the current-in-plane giant magnetoresistance (GMR) of a system consisting of a copper slab between two cobalt slabs, where the canting angle is the angle between the magnetization vectors of the two cobalt slabs. We utilize the layer-Kohn-Korringa-Rostoker method to self-consistently calculate the electronic structure. Electron scattering by impurities, phonons, magnons, etc., is modeled with a layer- and spin-dependent complex self-energy. Scattering rates are chosen to match Cu and Co resistivities. The scattering rate for minority Co is assumed to be seven times larger than for majority Co, the same ratio as for the Fermi energy density of states in the two channels. The nonlocal layer-dependent conductivity is calculated using the Kubo-Greenwood formula. We find that the GMR decreases with copper thickness in a nonuniform manner due to changes in the behavior of waveguidelike modes in the copper slab. For fixed copper thickness the GMR dependence on cos θ, where θ is the relative angle between the cobalt slabs magnetization directions, deviates from a linear dependence on cos θ.
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Since the 1988 discovery of giant magnetoresistance (GMR) in Fe/Cr multilayers,[1] intense interest has focused on this and similar systems in various geometries because of the technological promise of these materials as magnetic field sensors and possibly as novel spin effect transistors. Much of the early theoretical work in this area concentrated on free-electron models, and an extensive reference list is given in a recent review by Levy.[2] Within the free-electron model, Vedyayev *et al.*[3,4] investigated the angular dependence of the magnetoresistance. Experimentally, the limited data available[5,6] are consistent with a linear variation of the magnetoresistance with $1-\cos\theta$, where the canting angle θ is the relative angle between the directions of the moments in the ferromagnetic slabs.

In this paper we consider {111} fcc Co/Cu/Co in the spin valve geometry.[5] A spin valve consists of two ferromagnetic slabs separated by a nonmagnetic spacer slab. The magnetic moment direction of one of the ferromagnetic slabs is pinned by growing that layer on an antiferromagnet while the magnetic moment of the other ferromagnetic slab is free to rotate in response to a small to moderate external field. Previous first-principles calculations performed by Butler *et al.*[7] for Co/Cu multilayers and Co/Cu/Co spin valves revealed a pronounced nonlocal resonance effect between cobalt layers separated by a copper slab and an electron channeling effect (analogous to a waveguide) within the copper slab, but these calculations only included ferromagnetic ($\theta=0$) and antiferromagnetic ($\theta=\pi$) alignments of the moments and one spin valve thickness t (ten atomic {111} copper planes). This study examines the current-in-plane GMR dependence on t, and GMR calculations for fixed thickness t are displayed as a function of $1-\cos\theta$ for $t=7$.

The GMR is evaluated by first self-consistently calculating the electronic structure within the Layer-Kohn-Korringa-Rostoker (LKKR) formalism[8] with s, p, d, and f basis functions and ignoring spin-orbit coupling. For the self-consistency iterations, a spin valve of thickness t is modeled with an interface region of three cobalt, t copper, and three cobalt layers bounded by semi-infinite cobalt on both sides. The Fermi level of infinite cobalt fixes the Fermi level in the interface. At each iteration the potential in the entire interface region is shifted up or down as required to maintain charge neutrality. After self-consistency is achieved, spin- and layer-dependent scattering rates are introduced through the imaginary parts of the self-energies. They are chosen to yield correct Cu and Co resistivities in thick films. A spin asymmetry scattering rate factor of 7 in Co is consistent with the Fermi-level minority to majority density of states ratio. The scattering rates ($\hbar/\tau$), expressed in atomic Hartree units (1 aHu=27.2 eV), are 0.010 08 aHu for spin-up and 0.001 44 aHu for spin-down cobalt layers in the interface region, 0.000 60 aHu for spin-up and spin-down copper layers in the interface region, and no additional scattering at the interfacial boundaries. These scattering rates, when used with the calculated electronic structures of Co and Cu, yield resistivity values that match typical room temperature resistivities for thick sputtered films (2.8 $\mu\Omega$ cm for copper and 14.8 $\mu\Omega$ cm for cobalt). The semi-infinite regions on either side of the Co/Cu/Co interfacial region were modeled as Co, but with very large scattering rates of 0.2000 aHu for both spin up and spin down.

The nonlocal conductivity is given by the Kubo-Greenwood formula[9] as

$$\sigma_{mn}(\mathbf{r},\mathbf{r}')=\pi\hbar\langle j_m \,\mathrm{Im}\, G(E_F;\mathbf{r},\mathbf{r}')j_n \mathrm{Im}\, G(E_F;\mathbf{r}',\mathbf{r})\rangle, \tag{1}$$

where the angular brackets indicate a configurational average, j_μ is the current operator, and the Green function is

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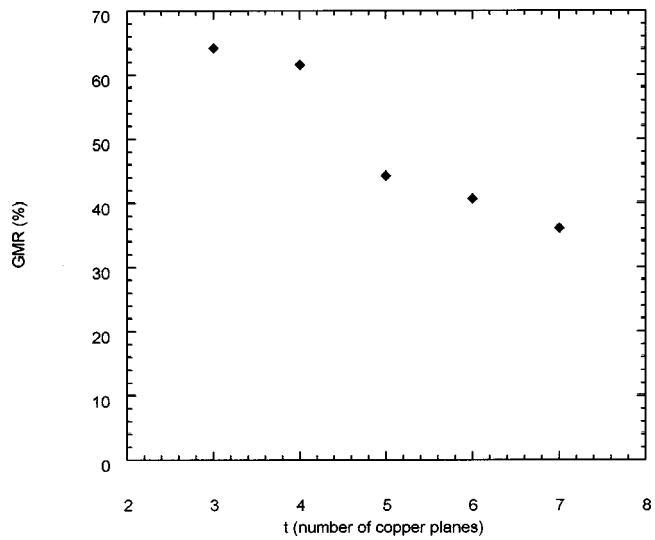

FIG. 1. GMR vs number of (111) copper planes (diamonds).

represented by a 2×2 nondiagonal matrix[10] to allow for canting angles other than 0 and π. In the evaluation of the configurational average, vertex corrections are neglected. Integrating over atomic cells in plane J and averaging over atomic cells in plane I generates the nonlocal layer conductivity[11] as

$$\sigma_{\mu\nu}(I,J)=N_I^{-1}\sum_i\sum_j\Omega_i^{-1}\int_{\Omega_i}d\mathbf{r}\int_{\Omega_j}d\mathbf{r}'\sigma_{\mu\nu}(\mathbf{r},\mathbf{r}'),\tag{2}$$

where $\sigma_{\mu\nu}(I,J)$ is the current in direction μ in atomic plane I due to an applied electric field of unit magnitude in direction ν applied in atomic plane J, N_I is the number of cells in plane I, and Ω_i is the volume of an atomic cell in plane i.

Figure 1 displays the dependence of the GMR on the thickness of the copper spacer layer. The GMR is calculated from the nonlocal conductivity by first summing over I and J and dividing by the number of layers to get the total conductivity $\sigma(\theta)$. Then

$$\mathrm{GMR}(\theta)=100\times\frac{\sigma(\theta)-\sigma(\pi)}{\sigma(\pi)}.\tag{3}$$

We believe that the precipitous decrease in GMR with increasing copper thickness between $t=4$ and 5 is an effect of the waveguide modes. In the simplest model these modes are free-electron-like in the (111) planes and standing waves perpendicular to the (111) planes. The modes can be labeled by the number of nodes inside the copper slab analogous to modes in the one-dimensional (1D) finite square well. Because the Fermi level is fixed, the lowest mode (with no nodes inside the well) occurs at the highest value of $\mathbf{k}_\parallel$ from $2E_F=\mathbf{k}_\parallel^2+\mathbf{k}_\perp^2$ in aHu with $\mathbf{k}_\parallel$ [parallel to (111) planes] and $\mathbf{k}_\perp$ [perpendicular to (111) planes] both real and positive inside the copper slab.

Although the conductivity consists of both on-site and nonlocal parts, examining just the on-site component gives insight into the conductivity behavior. For both ferromagnetic and antiferromagnetic alignments and for copper thicknesses from 3 to 6 atomic (111) planes, Fig. 2 shows the on-site conductivity $\sigma(I,I)$ in the 2D Brillouin zone along the Γ to $\bar{K}$ ray which forms one of the boundaries for the irreducible wedge for the inner most copper layer. From the zone boundary inward, it is possible to associate successive peaks with wave functions possessing an increasing number of nodes inside the copper slab starting with zero nodes for mode 1.

For example, for copper slabs with an odd number of layers, on-site conductivity contributions from even modes displayed in Fig. 2 tend to be suppressed on the central layer because of the presence of a node in the wave function. For copper slabs with an even number of layers, the suppression due to the central node of the even modes is moderated because it is shared by the two inner most copper layers. For $t=3$, 4, and 5 layers, three modes are discernible, and for $t=6$, four modes are evident. Similar results are obtained for other rays in the 2D Brillouin zone originating at Γ with the conductivity peak height decreasing as the chosen ray becomes farther from the Γ to $\bar{K}$ ray and finally vanishing completely near the other zone boundary due to the projection of a copper Fermi surface neck. When the integration is performed over the Brillouin zone, contributions from mode 1 dominate the conductivity.

The difference in the current carried by the channeling modes between the antiferromagnetic and ferromagnetic alignments is an important contributor to the GMR. Along Γ to $\bar{K}$ the ratio of the mode 1 antiferromagnetic to ferromagnetic peak height is 0.06, 0.13, 0.35, and 0.43 for $t=3$, 4, 5, and 6, respectively, with the smaller ratio indicating a larger contribution to the GMR. The largest increase in the ratio from $t=4$ to 5 corresponds to the jump in the GMR seen in Fig. 1. We speculate the the nonsmooth behavior described above is a characteristic of the presence of waveguide modes and may be observable experimentally in the thinnest and highest quality samples.

The nonsmooth behavior probably arises in the following way: for electron in a channeling mode, there are no majority Co states into which the electrons can refract and therefore they are totally reflected at the interface. For the minority electrons, however, there are states to refract into, and so there will not be perfect channeling. However, as the thickness of the spacer layer increases, the wavelength of the lowest channeling mode increases so that the perpendicular component of the momentum decreases and the parallel component increases so that the electrons in this mode are incident on the interface more nearly parallel to it. As the angle of incidence increases, there is a larger probability that the electron will reflect even off of the minority: thus the difference between the current carried in the channeling modes for ferromagnetic and antiferromagnetic alignment will decrease. This is illustrated in Fig. 3, which shows the calculated transmission coefficient of copper Bloch waves incident on minority cobalt decreasing as $\mathbf{k}_\parallel$ increases from 0.6 to 0.7 along Γ to $\bar{K}$.

Figure 4 presents the GMR angular dependence for $t=7$. At $\theta=\pi/2$ the calculated GMR is a smooth function and is reduced by about 30% from a simple linear dependence on $1-\cos\theta$. No comparable experimental data on Co/Cu/Co spin valves has been published to our knowledge. Previous

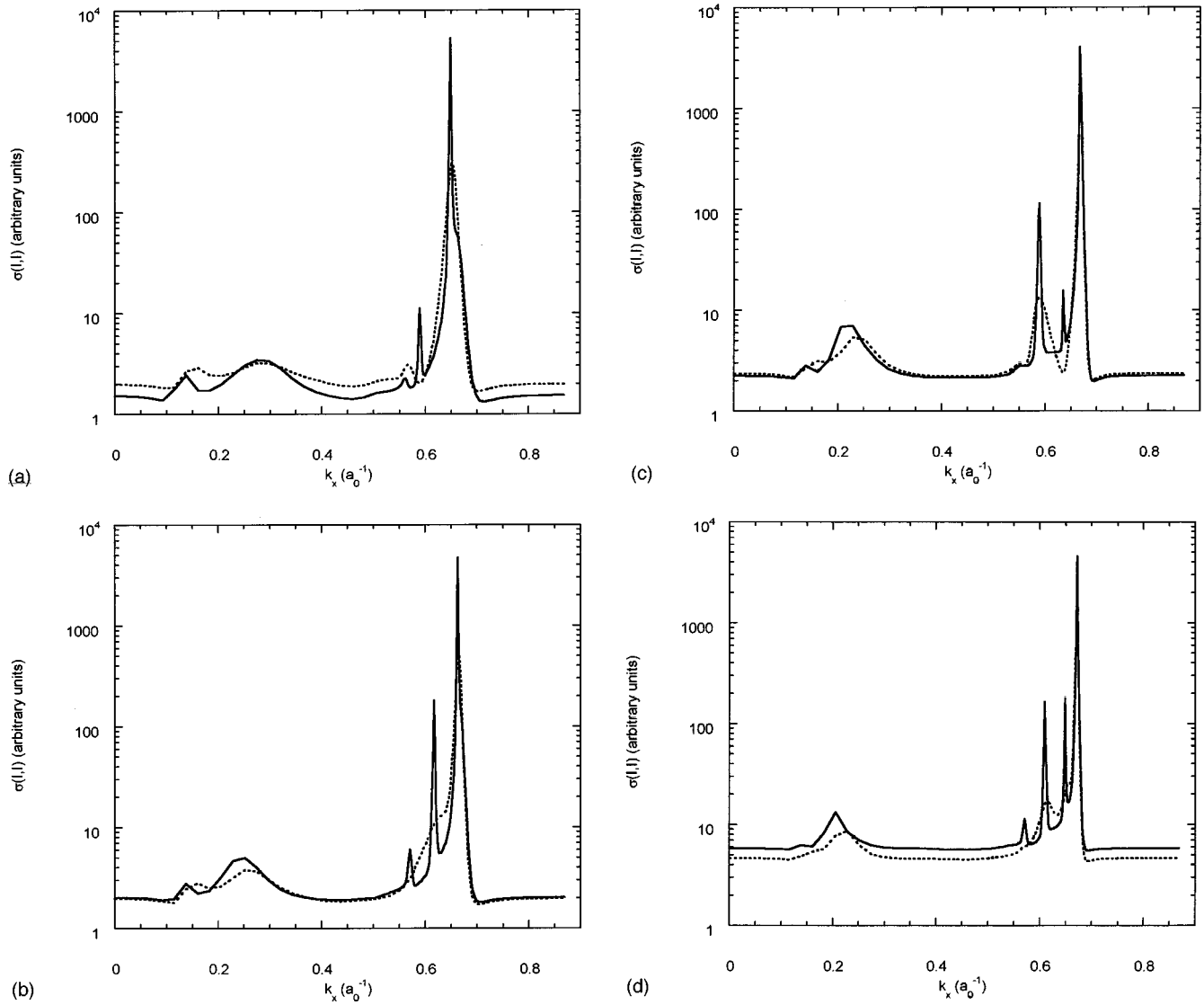

FIG. 2. On-site conductivity term vs $\mathbf{k}_{\parallel}$ from Γ to $\bar{K}$ for ferromagnetic (solid line) and antiferromagnetic alignments (dashed line): (a) interior copper plane for $t=3$, (b) interior copper plane for $t=4$, (c) second interior copper plane for $t=5$, and (d) second interior copper plane for $t=6$.

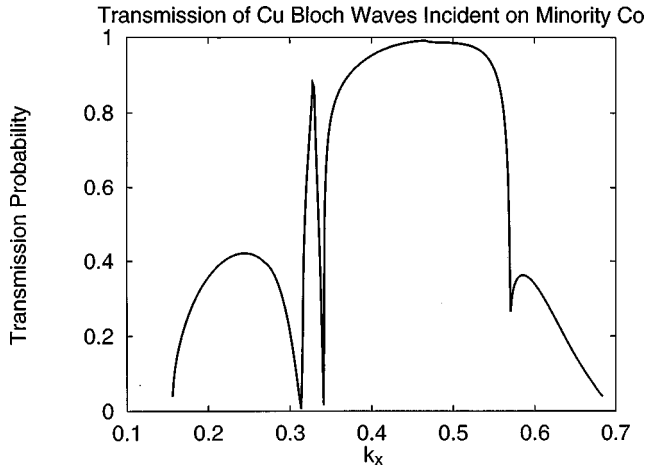

FIG. 3. Transmission probability of copper Bloch waves incident on minority cobalt versus k_x from Γ to $\bar{K}$.

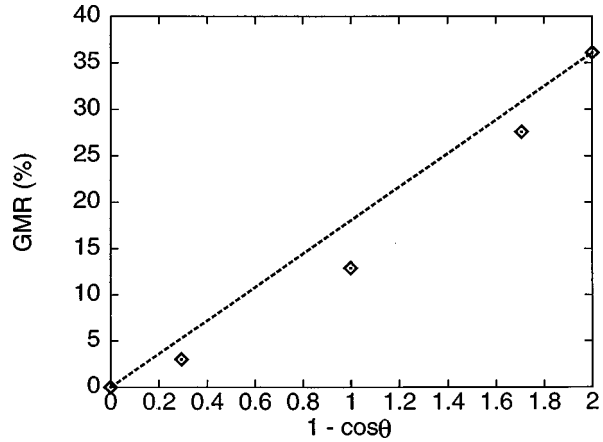

FIG. 4. GMR vs $1-\cos(\theta)$ (diamonds) for $t=7$ and a linear dashed line as a guide to the eye.

experimental measurements of the GMR angular dependence in NiFe/Cu/NiFe spin valves revealed no significant deviation from a linear dependence on $1-\cos\theta$.[5] Interfacial diffusion and roughness may have suppressed channeling contributions in these samples. In addition, no evidence is seen for spikes in the GMR(θ) as suggested by Vedyayev *et al.* due to a mechanism loosely analogous to the de Haas–van Alphen effect where increasing the thickness of the copper slab fills the role of the changing magnetic field. However, this calculation does not exclude that possibility because our grid in $1-\cos\theta$ is rather coarse and as such this comparison is indicative rather than definitive.

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