Calculation of the perpendicular giant magnetoresistance of Co/Cu(001) two-dimensional lateral superlattices

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The results of quantum calculations of the current-perpendicular-to-line giant magnetoresistance (CPL GMR) of Co/Cu(001) two-dimensional lateral superlattices are presented. They are obtained from an exact numerical evaluation of the Kubo formula using the electronic structures of Cu and Co monolayers described by s,p,d tight-binding bands. The calculations show that the CPL GMR of two Co wires separated by N atomic lines of Cu is strongly dependent on the Co wire widths and can be as large as 110%. The CPL GMR of finite, perfectly periodic Co/Cu(001) lateral superlattices is found to saturate after 5–6 repeats of the superlattice unit cell and reach a maximum value of $\approx$ 350%. Finally, the giant magnetoresistance ratios of superlattices with fluctuating Co wire widths are evaluated and shown to increase linearly with total superlattice length and be of the order of 1000% after 25 repeats of the superlattice unit cell. [S0163-1829(98)02606-X]

A sharp drop in the resistance of metallic magnetic multilayers occurs when the magnetizations of neighboring magnetic layers oriented spontaneously antiparallel are aligned in an applied saturating magnetic field. This so-called giant magnetoresistance (GMR) effect has received much attention.[1,2] GMR ratios as high as 200% have been reported in Fe/Cr superlattices,[3] holding the promise of potential applications in magnetic sensor technology. Most of the GMR experiments have been carried out in the current-in-plane (CIP) geometry in which the resistance of the multilayer is large and measurable with conventional techniques. This is because the length of the sample is much larger than the film thickness. By contrast, in the current-perpendicular-to-plane (CPP) geometry, the length of the sample is just the film multilayer thickness which is usually much smaller than its transverse dimensions. In this case the resistance can only be measured using very sensitive techniques. This can be achieved, for example, with superconducting contacts[4] but one problem that might arise are proximity effects. Alternatively, the resistance of the multilayer can be increased to easily measurable values by reducing the cross-sectional area of the sample to mesoscopic scale. Multilayer pillars of diameter as low as 60 nm have been fabricated by microlithography[5] leading to resistances of the order of mΩ which can be measured with conventional instruments.

The experimental trend is toward manufacturing structures of ever decreasing dimensions. Recent effort in nanofabrication technology[6] has focussed on the growth on stepped surfaces of lateral superlattices which are only a few atoms thick. Individual nanowires have already been grown successfully on a variety of substrates ranging from tungsten to silicon by decorating the step edges and the technology is being extended to the deposition of alternating wires of different metals with controlled widths and atomic-scale thicknesses.

From a theoretical point of view, small samples have the great advantage that, when their dimensions are smaller than the mean free path, impurity scattering becomes unimportant and the resistance (CPP GMR) can be calculated from first principles without any approximations. We have made such calculations for conventional multilayers[7–9] assuming that their transverse dimensions are small. The next logical step is to extend the calculations of CPP GMR to the two-dimensional nonmagnetic metallic structures incorporating magnetic wires that are now being manufactured experimentally. It is to be expected that impurity scattering in such quasi-two-dimensional systems is less important than in conventional three-dimensional magnetic multilayers but the quantum effects should be enhanced.

One inevitable consequence of nanowire deposition is that distances between wires cannot be controlled very precisely, which introduces randomness into the problem. Fortunately, this feature can be treated theoretically without any additional approximations and the effects of growth-induced fluctuations in wire position (width) on the GMR can be explored rigorously.

All the calculations presented in this paper are for a free-standing two-dimensional Co/Cu(001) lateral structure in the current-perpendicular-to-line (CPL) geometry. Such a structure should provide a reasonable approximation to a system of metallic wires deposited on an insulating substrate. Following our previous work on conventional magnetic multilayers,[7–9] we neglect impurity scattering and evaluate the CPL GMR due to quantum reflections from perfectly flat Co/Cu interfaces. CPP (CPL) transport measurements are usually made in the two-probe geometry and we therefore assume the superlattice to be sandwiched between two semi-infinite two-dimensional (2D) Cu lead wires with negligible resistances which play the roles of contacts. The calculations are based on an exact numerical evaluation of the Kubo formula using s,p,d tight-binding bands with hopping to first- and second-nearest neighbors.

First we show that the CPL-GMR of a two-dimensional structure containing two Co wires M atoms wide separated by N lines of Cu is strongly dependent on the width of the Co wires and reaches a maximum value of $\approx$ 110% comparable to the GMR of a conventional Co/Cu(001) trilayer[9] in the absence of impurity scattering. Due to the reduced dimensionality of the problem, the zero- and saturating-field resistances are now of the order of mΩ. In Refs. 7,8 Mathon predicted a large enhancement of the CPP GMR of conventional multilayers in which the layer thicknesses are allowed to deviate at random from their nominal values. We extend this work to two-dimensional structures and investigate the CPL GMR of finite 2D Co/Cu(001) superlattices with and without growth-induced fluctuations in wire widths. We show that the CPL GMR of finite, perfectly periodic 2D superlattices saturates after 5–6 repeats of the superlattice unit cell and can be as large as $\approx$ 350%. For superlattices with randomly fluctuating wire widths, we find a large enhancement of the GMR in accord with the predictions of Refs. 7,8 for conventional multilayers. For small fluctuations in wire widths we show that the zero- and saturating-field resistances follow Ohm's law as a function of total superlattice length. A detailed comparison with conventional multilayers is given.

The CPL GMR is defined in terms of the conductances for up- and down-spin electrons in the ferromagnetic (FM) and antiferromagnetic (AF) configurations of the magnetic wires 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 wires. Each of the conductances in Eq. (1) can be calculated at zero temperature from the Kubo formula[10] expressed in terms of one-electron Green's functions

$$\Gamma^{\sigma}=\frac{4e^2}{h}\sum_{k_{\parallel}}\ \mathrm{Re\ Tr}(\widetilde{G}^{\sigma}_{00}t^{\sigma}_{01}\widetilde{G}^{\sigma}_{11}t^{\sigma}_{10}-t^{\sigma}_{01}\widetilde{G}^{\sigma}_{10}t^{\sigma}_{01}\widetilde{G}^{\sigma}_{10}), \tag{2}$$

where we have taken the x axis parallel to the wires. Here as in Refs. 7–9, the indices 0 and 1 label the principal lines on the left and right of an imaginary cleavage plane separating the structure into two independent semi-infinite crystals and $\widetilde{G}_{ij}(k_x)=(1/2i)[G^{-}_{ij}(k_x)-G^{+}_{ij}(k_x)]$, where $G^{-}_{ij}(k_x)$ and $G^{+}_{ij}(k_x)$ are the matrix elements between principal lines i,j of the advanced and retarded Green's functions evaluated at the Fermi energy E_F. In Eq. (2), the trace is over all atomic orbital indices that are contained implicitly in the principal lines indices 0 and 1, the sum over k_x is over the one-dimensional Brillouin zone and t_{01} is the tight-binding hopping matrix between the principal lines 0 and 1.

The Green's functions required in Eq. (2) were calculated within our tight-binding model. Because second-nearest neighbors are included, each principal line contains two atomic lines and, therefore, all the Green's function and hopping matrices in Eq. (2) are 18×18 matrices. The most general structure we investigate consists of N_{rpt} repeats of a superlattice unit cell consisting of a ferromagnetic Co wire containing M_1 atomic lines followed by N atomic lines of Cu, then a second ferromagnetic wire with M_2 atomic lines

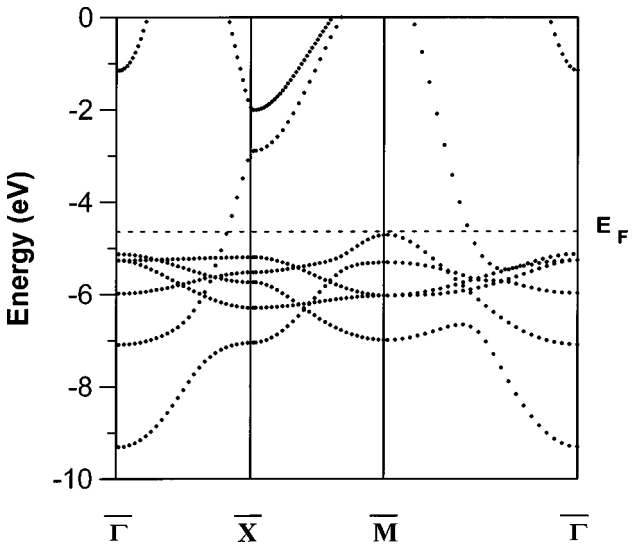

FIG. 1. Electronic structure of a Cu(001) monolayer along three high symmetry directions.

of Co and a second Cu wire with N atomic lines. The whole lateral structure is contained within an (001) atomic plane. In our tight-binding description, this means that electron hopping to neighboring (001) planes is terminated (free boundary conditions). The Co and Cu wires are described by tight-binding parameters for the respective free-standing monolayers, i.e., it is assumed that the interfaces between Co and Cu are abrupt. A small lattice mismatch between 2D Co and 2D Cu is neglected and the whole structure is taken to have the lattice parameter of 2D Cu.

The tight-binding parameters for two-dimensional Cu were determined from a fit to a first-principles electronic structure calculation[11] for a free-standing monolayer. Such a procedure was not feasible for two-dimensional ferromagnetic fcc Co as no *ab initio* band structure calculation could be found in the literature. In this case, the tight-binding parameters were obtained from paramagnetic 2D Cu, by self-consistently adjusting the on-site energies, assuming charge neutrality. The intra-atomic electron-electron interactions were taken to be $U^{\mathrm{Co}}_{sp}=0$ and $U^{\mathrm{Co}}_{d\text{-}d}=1$ eV and a magnetic moment of $2.07\mu_B$ was obtained. The hopping parameters were kept equal to those of 2D Cu. The magnetic moment we get is in reasonable agreement with the *ab initio* result ($1.90\mu_B$) of Noffke and Fritsche[12] for a monolayer cut out of hcp Co. To further check our approach, we have also applied it to 2D ferromagnetic Ni and, with parameters that fit the *ab initio* bands of Ref. 13, we obtained a magnetic moment of $0.95\mu_B$, in agreement with the results of Ref. 13. In our calculations we neglect the atomic potential difference due to the magnetic configuration, thereby making the approximation known as the ''force theorem.'' The band structures of 2D Cu and spin-polarized 2D Co, calculated with our sets of tight-binding parameters, are displayed in Figs. 1 and 2 for three high-symmetry directions.

The Green's functions $\widetilde{G}_{00},\widetilde{G}_{11},\widetilde{G}_{01}$ required in Eq. (2) are calculated in a manner similar to that described in Ref. 8. They are obtained from the surface Green's functions of the semi-infinite Cu lead wires using a one-dimensional analog of the method of adlayers.[14] The surface Green's functions of the left and right semi-infinite Cu leads are calculated using

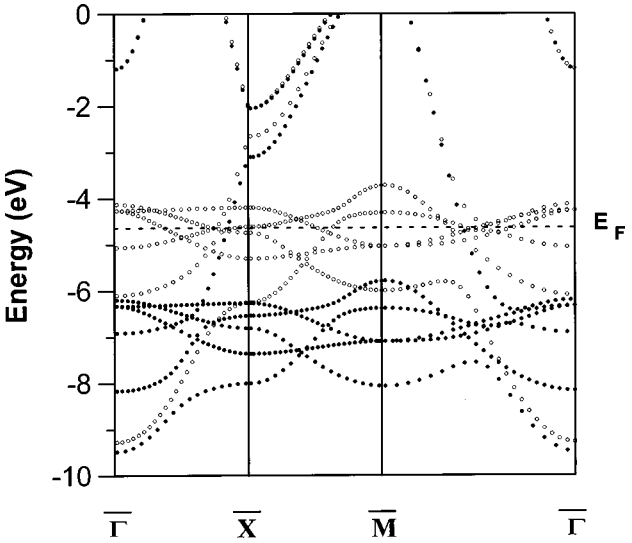

FIG. 2. Spin polarized energy bands of a fcc Co(001) monolayer along three high symmetry directions. The majority-spin bands are given by the full circles; open circles denote the minority-spin bands.

the noniterative technique of Umerski[15] in which a small imaginary part ($\epsilon = 10^{-8}$ Ry) is added to the energy to disrupt quantum interference effects between the two edges of the slab.

In all our calculations, the summation over k_x in Eq. (2) was carried out using 500 points in the one-dimensional Brillouin zone and convergence was checked by doubling the number of points taken in the sum. The choice of Cu wire width in all our samples was dictated by the requirement that the coupling between Co wires be antiferromagnetic. This happens, for example, for Cu wires containing seven atomic lines and all the results presented below will have $N_{\mathrm{Cu}} = 7$.

We first calculate the CPL GMR ratio of a single superlattice unit cell with equal Co wire widths $M_1 = M_2 = M$. A strong dependence on Co wire width is obtained as can be seen from Fig. 3. The CPL GMR ratio oscillates between some 40 and 110 % depending on Co thickness. These oscillations are due to quantum interferences from electron waves

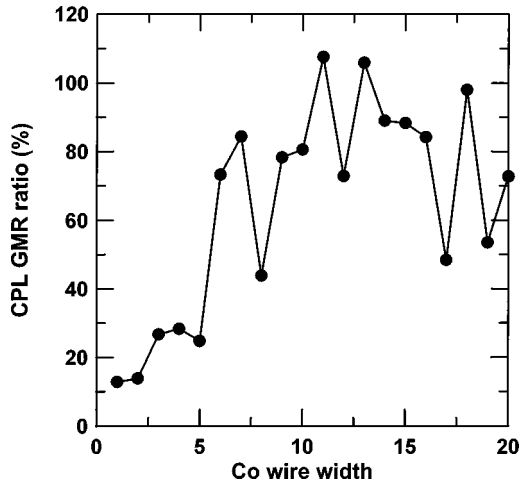

FIG. 3. Cobalt-thickness dependence of the CPL GMR ratio of a system consisting of two Co wires separated by seven lines of Cu.

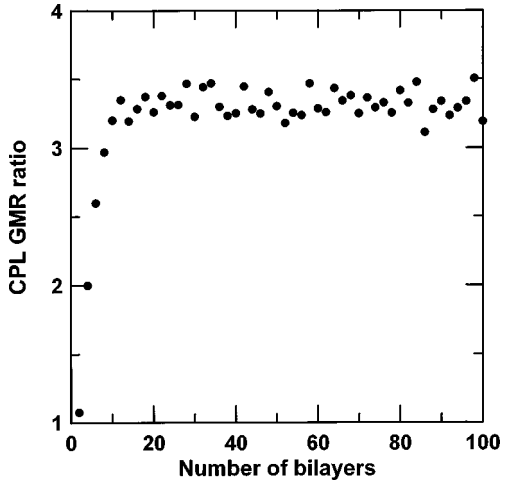

FIG. 4. Dependence of the CPL GMR ratio of a finite Co(11)/Cu(7) superlattice on the number of bilayers N_b.

scattered from the flat Co/Cu interfaces and the large oscillation amplitude indicates that the magnetic contrast is more marked than in conventional Co/Cu(001) trilayers. Indeed it can be seen from Figs. 1 and 2 that the majority spin bands of 2D Co and Cu are well matched while there is a large band offset for the minority spin bands. This is confirmed by the values of the ballistic conductances of bulk 2D Cu and spin-polarized 2D Co calculated at the Fermi energy from the Kubo formula. The conductance (per atom) at E_F for the majority spin channel of ferromagnetic fcc 2D Co is $1.17e^2/h$, close to that of 2D Cu ($1.14e^2/h$). The conductance for the minority spin channel of 2D Co is much larger $2.97e^2/h$, as the Fermi energy falls deep into the d band of 2D Co.

Figure 4 shows the dependence of the CPL GMR ratio on the number of bilayers ($N_b = 2N_{\mathrm{rpt}}$) in a finite, perfectly periodic Co/Cu(001) lateral superlattice with fixed Co and Cu wire widths. As before, $N_{\mathrm{Cu}} = 7$ and the number of atomic lines in the Co wires was set equal to $M_1 = M_2 = 11$, for which a large GMR ratio is obtained when $N_{\mathrm{rpt}} = 1$ (see Fig. 3). The CPL GMR ratio is seen to saturate after only 5–6 repeats (10–12 bilayers) of the superlattice unit cell and the GMR is enhanced by a factor 3–4 compared to that of $N_{\mathrm{rpt}} = 1$, reaching a maximum saturation value of 350%. A similar enhancement factor is obtained for other Co and Cu wire widths. The enhancement is larger than in conventional three-dimensional perfectly periodic Co/Cu (001) superlattices for which the maximum CPP GMR ratio was found to be around 150%. This is due entirely to the differences in electronic structure between the 2D and 3D cases and reflects again the larger magnetic contrast discussed above for the 2D case.

Finally, we investigate the case in which the Co wire widths fluctuate at random from their nominal values by no more than one atomic line. The number of Co atomic lines is chosen to follow a pseudorandom sequence of integers M_i, generated over the interval $[M_{\min}, M_{\max}]$, with $M_{\max} - M_{\min} = 1$. Results are shown in Figs. 5 and 6 for a superlattice with $M_{\min} = 5$ and $M_{\max} = 6$. The zero- and saturating-field resistances R_{AF} and R_{FM} displayed in Fig. 5 increase linearly with total superlattice length (Ohm's law) but the rate of increase is slower than in conventional superlattices

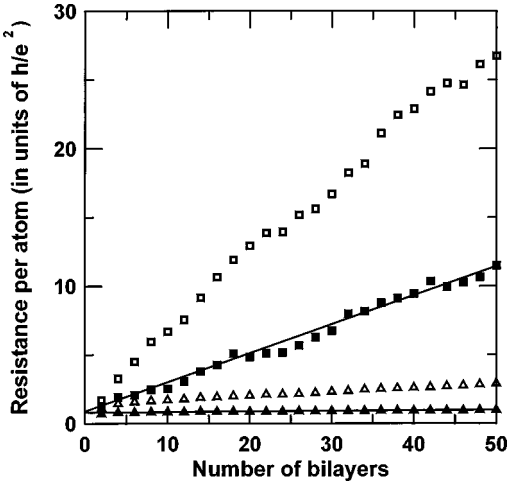

FIG. 5. Total resistances R_{AF} and R_{FM} in the antiferromagnetic (AF) and ferromagnetic (FM) configurations of conventional (open symbols) and lateral (full symbols) Co(5–6)/Cu(7) superlattices with small fluctuations in Co thickness plotted against the number of bilayers N_b. Squares denote the resistance R_{AF} and triangles the resistance R_{FM}. The straight lines are a guide to the eye.

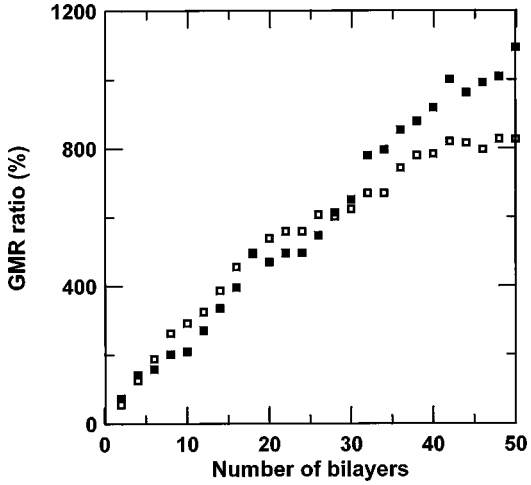

FIG. 6. CPP (CPL) GMR ratio of conventional (open squares) and lateral (full squares) Co(5–6)/Cu(7) superlattices with small fluctuations in Co thickness plotted against the number of bilayers N_b.

with comparable spacer and ferromagnet thicknesses. However, the GMR ratios are very similar in both cases (Fig. 6) and increase linearly with the number of bilayers N_b. For larger N_b, the CPP GMR of conventional superlattices reaches a saturation value. For lateral superlattices such a saturation was not obtained as localization sets in before the saturation can be reached. As in Ref. 8 it was checked that the calculated conductances are insensitive to the choice of pseudorandom sequence used for M_i and therefore an average over configurations is not required.

In conclusion, we have investigated the transport properties of Co/Cu(001) lateral superlattices in the perpendicular geometry. We have neglected the effect of impurities and obtained the contribution to the GMR due to quantum scattering of the electron waves at the Co/Cu interfaces. The quantum interference effects are more pronounced than in conventional magnetic multilayers leading to a stronger dependence of the GMR on Co wire width. Suitable choice of Co and Cu wire widths allows tuning of the GMR to a maximum value of $\approx$ 110% for a Co/Cu/Co sandwich and $\approx$350% for a finite, perfectly periodic Co/Cu(001) lateral superlattice. The latter is much larger than the maximum CPP GMR of conventional Co/Cu(001) periodic superlattices which was found to be around 150%. Finally, for superlattices in which the Co wire widths deviate at random from their nominal value by a small amount we found that the GMR ratios increase linearly with total superlattice length and reach values of order 1000% after 25 repeats of the superlattice unit cell, comparable to the values obtained for conventional multilayers with random fluctuations in layer thicknesses. The zero- and saturating-field resistances approximately follow Ohm's law and are now of the order of mΩ. It follows that the voltage drop on such samples would be much larger than for conventional multilayers and should therefore be more easily measurable. All these results were obtained for free-standing lateral structures and should remain valid qualitatively for nanowires on insulating substrates.

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[1] M. N. Baibich, J. M. Broto, A. Fert, F. Van Dau Nguyen, F. Petroff, P. Etienne, G. Creuzet, A. Friederich, and J. Chazelas, Phys. Rev. Lett. **61,** 2472 (1988); G. Binasch, P. Grünberg, F. Saurenbach, and W. Zinn, Phys. Rev. B **39**, 4828 (1989); S. S. P. Parkin, N. More, and K. P. Roche, Phys. Rev. Lett. **64**, 2304 (1990).

[2] M. A. M. Gijs and G. E. W. Bauer, Adv. Phys. **46**, 285 (1997).

[3] R. Schad, C. D. Potter, P. Belien, G. Verbanck, V. V. Moschchalkov, and Y. Bruynseraede, Appl. Phys. Lett. **64**, 3500 (1994).

[4] W. P. Pratt, Jr., S.-F. Lee, J. M. Slaughter, R. Loloee, P. A. Schroeder, and J. Bass, Phys. Rev. Lett. **66**, 3060 (1991).

[5] M. A. M. Gijs, S. K. Lenczowski, and J. B. Giesbers, Phys. Rev. Lett. **70**, 3343 (1993).

[6] T. Jung, R. Schlittler, J. K. Gimzewski, and F. J. Himpsel, Appl. Phys. A: Solids Surf. **61**, 467 (1995); F. J. Himpsel, Bull. Am. Phys. Soc. **42**, 92 (1997).

[7] J. Mathon, Phys. Rev. B **54**, 55 (1996).

[8] J. Mathon, Phys. Rev. B **55**, 960 (1997).

[9] J. Mathon, A. Umerski, and M. Villeret, Phys. Rev. B **55**, 14 378 (1997).

[10] P. A. Lee and D. S. Fisher, Phys. Rev. Lett. **47**, 882 (1981).

[11] O. Jepsen, J. Madsen, and O. K. Andersen, Phys. Rev. B **18**, 605 (1978); J. R. Smith, J. G. Gay, and F. J. Arlinghaus, *ibid.* **21**, 2201 (1980); G. S. Painter, Phys. Rev. B **17**, 3848 (1978).

[12] J. Noffke and L. Fritsche, J. Phys. C **14**, 89 (1981).

[13] Xue-Yuan Zhu and J. Hermanson, Phys. Rev. B **27**, 2092 (1983).

[14] J. Mathon, J. Phys.: Condens. Matter **1**, 2505 (1989).

[15] A. Umerski, Phys. Rev. B **55**, 5266 (1997).