

Giant magnetoresistance of repeated multilayers of Cu_3Ni_3 embedded in Cu(100)

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ABSTRACT

The resistivity and giant magnetoresistance (GMR) of $(\text{Cu}_3\text{Ni}_3)_n$ embedded in Cu(100), for $n \leq 11$, that originates from the electronic structure of these finite, yet otherwise perfect, systems is calculated for currents in the plane of the layers (CIP) by using the Kubo–Greenwood formula for semi-infinite systems and the fully relativistic, spin-polarized screened Korringa–Kohn–Rostoker method. We find that for this particular type of repeated structure the CIP resistivity decreases from about 6 to $2 \mu\Omega \text{ cm}$ as the number of repeats increases from 2 to 11, and the CIP-GMR while starting out at 4% for $n=2$ goes up to 16% at $n=11$.

§1. INTRODUCTION

We have developed a method to calculate the conductivity (resistivity) and giant magnetoresistance (GMR) of finite layered structures that is based on the Kubo–Greenwood formalism (see Butler (1985) and Banhart (1998)). Our approach is able to correctly account for the resistance coming from defects as well as that intrinsic to a finite layered structure (see Blaas *et al.* (1998a,b)). As we increase the number of repeats n of a basis, e.g. Cu_3Ni_3 , the expectation is that the electronic structure—and also resistivity and GMR—for the multilayer will approach that of an infinitely translationally invariant system with this basis provided n is large enough. We have calculated the resistivity and GMR for a series of layered structures $(\text{Cu}_3\text{Ni}_3)_n$, with $n \leq 11$, for currents in the plane of the layers (CIP); here we limit ourselves to otherwise perfect structures (no defects) and therefore to intrinsic sources of resistance and GMR. Intrinsic sources are: the ‘confinement’ resistance for a finite but otherwise perfect structure, and differences in the electronic structures for the parallel (P) and antiparallel (AP) alignments of the moments in adjacent magnetic slabs which produce GMR (see Schep *et al.* (1995, 1998)). As n increases we find, as expected, the intrinsic resistivity (i.e. the resistance divided by the number of layers) decreases and the GMR increases. However, we are limited at the present

time to a rather small number of repeats $n \leq 11$ because of the computational effort; therefore we are unable to determine whether the intrinsic resistivity, i.e. the resistance divided by the number of layers or repeats, of $(\text{Cu}_3\text{Ni}_3)_n$ goes to zero as n goes to infinity.

§2. THEORETICAL DESCRIPTION

By using the so-called Kubo–Greenwood formula (Kubo 1957, Greenwood 1958) the electrical conductivity of a system, namely $\sigma_{\mu\mu}$, is given by

$$\sigma_{\mu\mu} = \frac{\pi\hbar}{N_0\Omega_{\text{at}}} \left\langle \sum_{m,n} J_{mn}^{\mu} J_{nm}^{\mu} \delta(\epsilon_{\text{F}} - \epsilon_m) \delta(\epsilon_{\text{F}} - \epsilon_n) \right\rangle. \quad (1)$$

In this equation $\mu \in \{x, y, z\}$, N_0 is the number of atoms, Ω_{at} is the atomic volume, J^{μ} is a representation of the μ th component of the current operator,

$$J^{\mu} = \{J_{nm}^{\mu}\}; \quad J_{nm}^{\mu} = \langle n | J_{\mu} | m \rangle, \quad (2)$$

with $|m\rangle$ describing the eigenstates of a particular configuration of the random system, ϵ_{F} is the Fermi energy, and $\langle \dots \rangle$ denotes an average over configurations. Equation (1) can be re-formulated in terms of the imaginary part of the (one-particle) Green's function G (see Butler (1985) or Banhart (1998)),

$$\sigma_{\mu\mu} = \frac{\hbar}{\pi N_0 \Omega_{\text{at}}} \text{Tr} \langle J_{\mu} \text{Im} G^+(\epsilon_{\text{F}}) J_{\mu} \text{Im} G^+(\epsilon_{\text{F}}) \rangle, \quad (3)$$

or by using ‘up-’ and ‘down-’ side limits, this equation can be re-written as

$$\sigma_{\mu\mu} = \frac{1}{4} \{ \tilde{\sigma}_{\mu\mu}(\epsilon^+, \epsilon^+) + \tilde{\sigma}_{\mu\mu}(\epsilon^-, \epsilon^-) - \tilde{\sigma}_{\mu\mu}(\epsilon^+, \epsilon^-) - \tilde{\sigma}_{\mu\mu}(\epsilon^-, \epsilon^+) \}, \quad (4)$$

where

$$\epsilon^+ = \epsilon_{\text{F}} + i\delta, \quad \epsilon^- = \epsilon_{\text{F}} - i\delta; \quad \delta \rightarrow 0, \quad (5)$$

and

$$\tilde{\sigma}_{\mu\mu}(\epsilon_1, \epsilon_2) = - \frac{\hbar}{\pi N_0 \Omega_{\text{at}}} \text{Tr} \langle J_{\mu} G(\epsilon_1) J_{\mu} G(\epsilon_2) \rangle; \quad \epsilon_i = \epsilon^{\pm}; \quad i = 1, 2. \quad (6)$$

It was shown in quite some detail by Butler *et al.* (1994) and Weinberger *et al.* (1996) that for layered systems, i.e. systems characterized only by two-dimensional translational symmetry, equation (6) is of the form

$$\tilde{\sigma}_{\mu\mu}(\epsilon_1, \epsilon_2) = \sum_{p,q=1}^L \tilde{\sigma}_{\mu\mu}^{pq}(\epsilon_1, \epsilon_2), \quad (7)$$

where L is the number of layers in the multilayer system to be summed over. $\sigma_{\mu\mu}^{pq}$ is calculated from $\tilde{\sigma}_{\mu\mu}^{pq}(\epsilon_1, \epsilon_2)$ by using equation (4) and denotes the conductivity that describes the current in layer p caused by an electric field in layer q .

§3. RESULTS AND DISCUSSION

In the present paper repeats of Cu_3Ni_3 embedded in Cu(100) are investigated (see also Zabloudil *et al.* (1998))

$$\begin{array}{ccccccccccc}
 \text{Cu}(100) \text{ Cu}_3 \parallel & \text{Ni}_3 & \text{Cu}_3 & \text{Ni}_3 & \text{Cu}_3 & \text{Ni}_3 & \text{Cu}_3 & \cdots & \text{Ni}_3 & \parallel & \text{Cu}_3 \text{ Cu}(100) \\
 \text{parallel(P)} & \rightarrow & & \rightarrow & & \rightarrow & & & \rightarrow & & \\
 \text{antiparallel(AP)} & \rightarrow & & \leftarrow & & \rightarrow & & & \leftarrow & &
 \end{array} \quad (8)$$

in which the various planes of the multilayer refer to the parent lattice of fcc Cu at the experimental lattice spacing. In the case of the **P** (parallel or ferromagnetic) arrangement all orientations of the effective magnetization in the magnetic Ni layers point along the surface normal, while in the **AP** (antiparallel or antiferromagnetic) arrangement the orientation of the effective magnetization is of opposite direction in every other set of Ni layers. As can be easily seen from the scheme in equation (8) we sum up only between the outermost Ni layers, and the total number of layers L to be summed over in equation (7) for a particular multilayer system is therefore given by $L = (6n - 3)$, where n is the number of repetitions.

All calculations reported here are based on the fully relativistic, spin-polarized screened Korringa–Kohn–Rostoker method for generating the corresponding self-consistent scattering potentials (see Zablouil *et al.* (1998)), as well as for the evaluation of the electrical conductivity tensor for which 990 \mathbf{k}_{\parallel} points in the irreducible wedge of the surface Brillouin zone are used.

To keep the time for the calculations reasonable we used a rather large value for the imaginary part of the energy in the calculations of the propagators: 5 mRyd (an even larger number of \mathbf{k}_{\parallel} points would have been necessary for computations with a smaller imaginary part of the energy). As one should be evaluating the propagators on the real axis, i.e. in the limit $\delta \rightarrow 0$ in equation (5), this introduces a spurious source of resistivity in the calculations that should be removed. We have done this by evaluating the resistivity again for $n=5$ and $n=6$ by using smaller values for the imaginary part of the energy, and then by extrapolation finding a correction that allows us to determine the resistivity we would have found had we been on the real axis. In our previous work we determined the resistivity of pure, yet finite, copper and cobalt (see Blaas *et al.* (1998a,b)), where the corrected resistivities gave as expected a confinement resistance and zero resistivity in the limit as the number of layers went to infinity. In our current analysis we followed the same procedure, however we are limited to $n \leq 11$ repeats of the basis Cu_3Ni_3 , which actually corresponds to only five repeats in the **AP** configuration. In the previous studies on copper and cobalt we had about 40 repeats of the basis, and it seems that the present number of repeats is insufficient for a reliable extrapolation as n goes to infinity.

Figure 1 shows the CIP resistivity $\rho_{xx}^{\alpha} = \rho_{yy}^{\alpha}$ (with $\rho_{\mu\mu}^{\alpha} = 1/\sigma_{\mu\mu}^{\alpha}$) of $(\text{Cu}_3\text{Ni}_3)_n$ multilayers embedded in $\text{Cu}(100)$, where α refers to **P** or **AP** alignments of the moments in neighbouring sets of Ni layers. As expected the resistivity decreases as the number of repeats increases, the CIP resistivity decreases from about 6 to $2 \mu\Omega \text{ cm}$ as the number of repeats n increases from 2 to 11. The CIP-GMR, defined as $(\rho_{xx}^{\text{AP}} - \rho_{xx}^{\text{P}})/\rho_{xx}^{\text{AP}}$, is shown in figure 2. While starting out at 4% for $n=2$ it goes up to 16% at $n=11$, and saturates at a higher GMR ratio only for considerably larger numbers of repeats n . At this time we are unable to check this saturation behaviour because of the computational effort.

In figures 3 and 4 we illustrate the layer-resolved contributions to the CIP conductivity σ_{xx}^{pq} for the case of $n=4$, namely for $(\text{Cu}_3\text{Ni}_3)_4$ embedded in $\text{Cu}(100)$. It is evident that the main contributions to σ_{xx} are located in the (pq) -plane at or near the diagonal $q=p$. For larger differences $q-p$ the contributions to σ_{xx} fall off quite

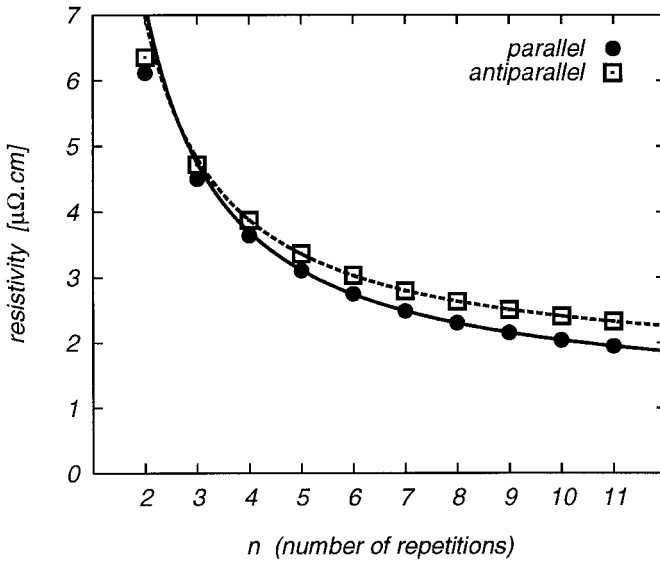


Figure 1. CIP resistivity ρ_{xx} of $(\text{Cu}_3\text{Ni}_3)_n$ multilayers embedded in Cu(100) for parallel and antiparallel alignments of moments in adjacent sets of magnetic Ni layers displayed versus the number of repetitions n .

rapidly: for example, for $q - p = 9$, $\sigma_{xx}^{pq} \leq 0.03$ au, which is already well below 5% of the largest contributions at $q = p$. The influence of the finite size of the system clearly shows up in the reduced conductivity contribution coming from the outermost Ni layers, see figure 4(a). The contributions from inside the multilayer are higher and relatively independent on the number of repetitions n . This peculiar structure results from the formation of quantum well and interface states in layered structures (see

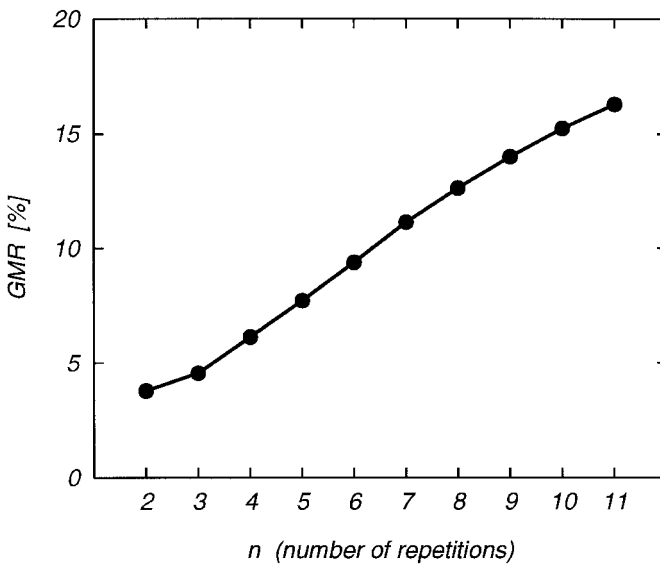


Figure 2. In-plane giant magnetoresistance (CIP-GMR) of $(\text{Cu}_3\text{Ni}_3)_n$ multilayers embedded in Cu(100) as a function of the number of repetitions n .

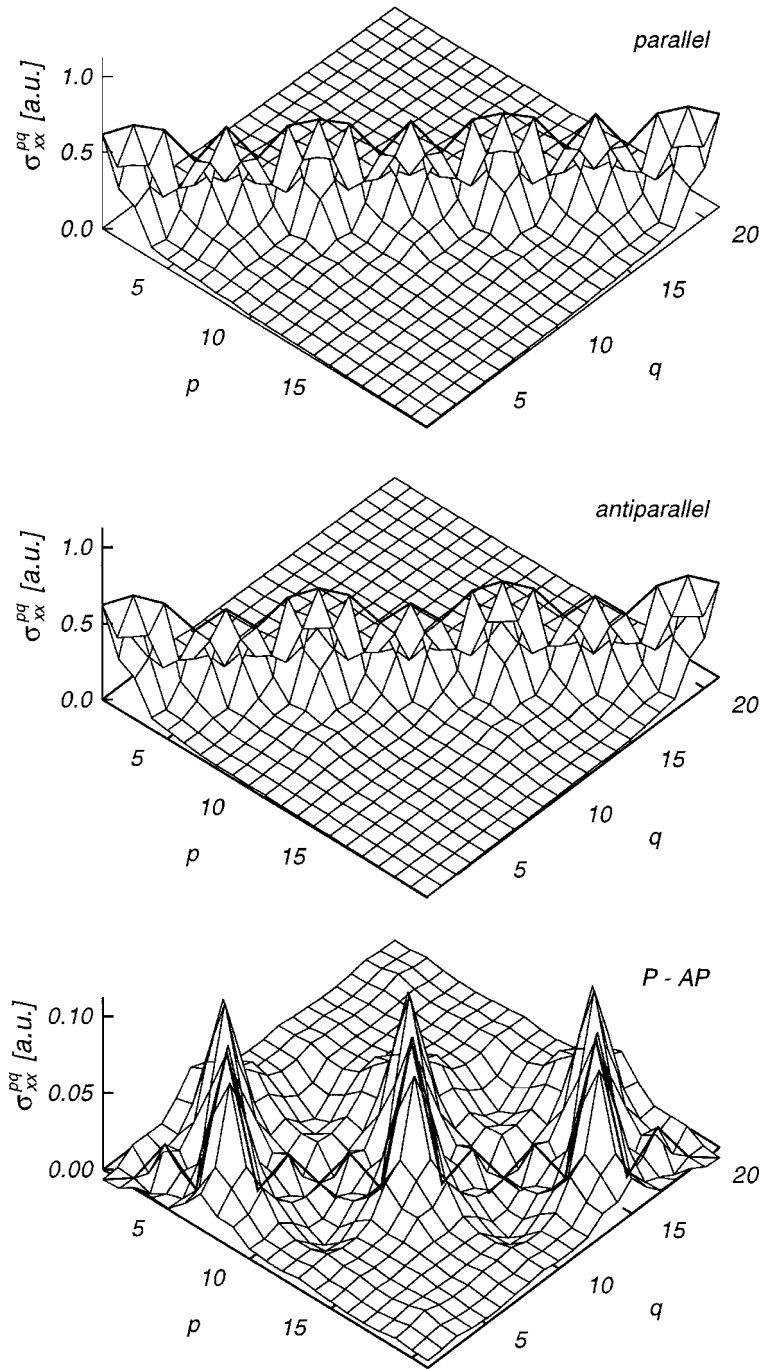


Figure 3. Layer-resolved contributions to the conductivity σ_{xx}^{pq} for $(\text{Cu}_3\text{Ni}_3)_4$ embedded in $\text{Cu}(100)$ for parallel (top) and antiparallel (middle) alignments of moments in adjacent sets of magnetic Ni layers. The difference between P and AP configurations (bottom) is also shown. For matters of convenience the diagonal elements (i.e. those for $q = p$, compare also to figure 4(b)) are connected by a thick full line. Ni layers are at $p, q = 1-3, 7-9, 13-15, \text{ and } 19-21$, respectively.

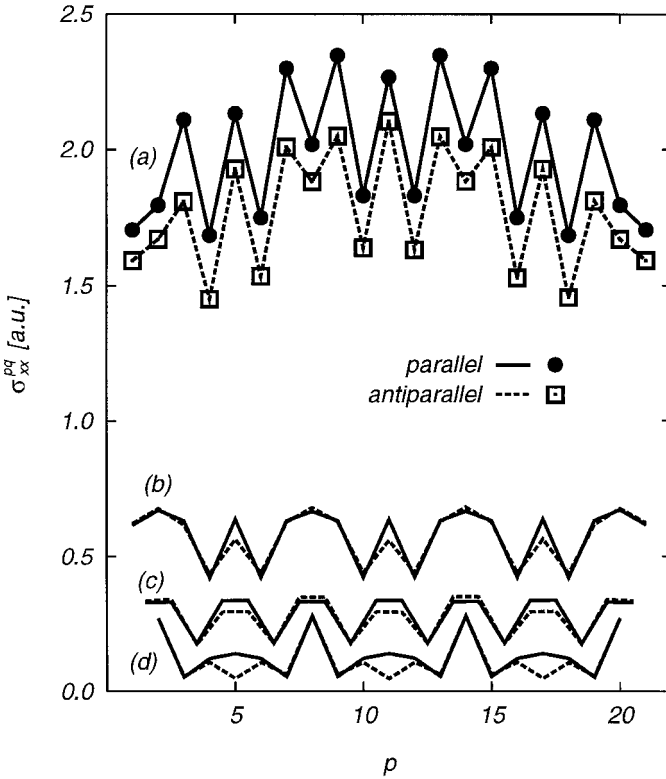


Figure 4. Layer-resolved contributions to the conductivity σ_{xx}^{pq} for $(\text{Cu}_3\text{Ni}_3)_4$ embedded in $\text{Cu}(100)$ for parallel and antiparallel alignments of moments in adjacent sets of magnetic Ni layers displayed versus the layer index p or versus $p + (p - q)/2$. (a) gives the result of the summation over one index q , i.e. $\sum_{q=1}^L \sigma_{xx}^{pq}$, while the individual contributions σ_{xx}^{pq} are displayed for (b) $q = p$, (c) $q = p - 1$, and (d) $q = p - 2$, respectively.

Zahn *et al.* (1998)). The differences of layer-resolved conductivities between P and AP configurations (shown in figure 3) demonstrates that the contributions of the Cu layers and of the Ni interface layers are extremely important for producing the GMR effect. These differences are caused by the absence of the highly conducting quantum well states in the AP configuration as compared to those present in the P configuration.

In conclusion it is important to stress that we have found only the resistivity and GMR arising from intrinsic sources, i.e. from the fact that the systems we are studying are finite, and from differences in the electronic structures for the parallel and antiparallel alignments of the moments in adjacent magnetic layers. We have not yet introduced impurities for the multilayers studied in the present paper (in our method it is indeed possible to simultaneously evaluate the resistivity and GMR arising from the electronic structure and from impurity scattering on an *ab initio* level as discussed by Blaas *et al.* (1998a,b)). Therefore we cannot compare our results presented here to data on real structures where the transport is diffusive and limited by scattering from impurities. Depending on the relative amount of spin-dependent to spin-independent scattering by impurities the GMR of real structures can be enhanced or reduced relative to the intrinsic values we have calculated here.

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