Electrical transport properties of bulk Ni_cFe_{1-c} alloys and related spin-valve systems

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Within the Kubo-Greenwood formalism we use the fully relativistic, spin-polarized, screened Korringa-Kohn-Rostoker method together with the coherent-potential approximation for layered systems to calculate the resistivity for the permalloy series Ni_cFe_{1-c}. We are able to reproduce the variation of the resistivity across the entire series; notably the discontinuous behavior in the vicinity of the structural phase transition from bcc to fcc. The absolute values for the resistivity are within a factor of 2 of the experimental data. Also the giant magnetoresistance of a series of permalloy-based spin-valve structures is estimated; we are able to reproduce the trends observed on prototypical spin-valve structures.

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I. INTRODUCTION

Permalloy is perhaps the most commonly used magnetic material in a variety of devices. This arises primarily from its magnetic properties which combine a reasonably high magnetic moment with a low coercivity. In many of its applications one passes a current through the material, so that its electrical transport properties are also important. There have been several calculations of the transport properties of permalloy, but none has been completely successful. Therefore, one of the outstanding challenges has been an *ab initio* calculation of the electrical resistivity and anisotropic magnetoresistance across the entire Ni_cFe_{1-c} series. Here we present the first part which addresses the resistivity of bulk permalloy and also the giant magnetoresistance of spin-valve structures containing layers of permalloy. As the lattice structure changes from bcc to fcc at $c \simeq 35\%$ we present results for both lattice structures. We are able to reproduce the overall variation of the resistivity across the series; in particular we find the signature changes in resistivity about $c \simeq 35\%$ as the lattice structure changes from bcc to fcc. Remarkably we find the magnitude of the resistivity is within a factor of 2 of the experimental values; noteworthy our calculated values are larger, so that when one relaxes the approximations we made one reduces the resistivities and approaches the measured ones.

Here we outline our *ab initio* calculation and present our results for the resistivity across the entire Ni_cFe_{1-c} series. Then we conclude with results on prototypical spin-valve structures containing permalloy layers, e.g., Ni_cFe_{1-c}(100 Å)/Co(6 Å)/Cu(9 Å)/Co(6 Å)/Ni_cFe_{1-c}(5 Å). Here we find trends in the current in the plane of the layers (CIP) magnetoresistance ratios that compare favorably with those observed in similar structures.

II. METHOD OF CALCULATION

In terms of the Kubo-Greenwood approach for disordered layered systems with growth direction along the surface normal (z axis) the in-plane conductivity is given by[1]

$$\sigma_{\mu\mu}(n;\mathbf{c};\mathcal{C}) = \sum_{i,j=1}^{n} \sigma_{\mu\mu}^{ij}(\mathbf{c};\mathcal{C}), \quad \mu \in \{x,y\},$$

$$\sigma_{\mu\mu}^{ij} = \frac{\hbar}{\pi N_0 \Omega_{\mathrm{at}}} \mathrm{Tr}\langle J_\mu^i \mathrm{Im}G^+(\epsilon_F) J_\mu^j \mathrm{Im}G^+(\epsilon_F)\rangle, \qquad (1)$$

where n denotes the number of layers considered, $\mathbf{c} = \{c_1, c_2, \ldots, c_n\}$ is a set containing the layerwise compositions, e.g., the layerwise concentrations in an inhomogeneously disordered binary alloy system $A_{c_i}B_{1-c_i}$ (in a homogeneously disordered alloy $c_i = c, \forall i$; whereas in a spin-valve system $A_m/B_n/A_m$ the $c_i = 1, \forall i \in A_m$, and $c_i = 0, \forall i \in B_n$). In principle the magnetization in each layer of a multilayered structure can be different, and $\mathcal{C} = \{\mathbf{M}_1, \mathbf{M}_2, \ldots, \mathbf{M}_n\}$ denotes a particular magnetic configuration, where the $\mathbf{M}_i$ refer to the orientations of the magnetizations in the individual layers. $\sigma_{\mu\mu}^{ij}$ is the conductivity that describes the current in layer i caused by an electric field in layer j, N_0 the number of atoms per plane of atoms, Ω_{at} is

the atomic volume, $\langle \cdots \rangle$ denotes an average over configurations, J_μ^i is the μth component of the current operator referenced to the ith plane, and G^+ is the electron propagator (one-particle Green's function) from plane i to j at the Fermi energy ϵ_F. The resistivity corresponding to the conductivity given by Eq. (1) is then defined by

$$\rho_{\mu\mu}(n;\mathbf{c};\mathcal{C}) = 1/\sigma_{\mu\mu}(n;\mathbf{c};\mathcal{C}), \quad \mu \in \{x,y\}. \tag{2}$$

This expression is restricted to CIP; for currents perpendicular to the planes of layers (CPP) the resistivity for a finite layered structure cannot be written in this way (see Ref. 2). By assuming two different magnetic configurations, $\mathcal{C}$ and $\mathcal{C}'$, the relative change in the resistivities between them is given by the ratio

$$R_{\mu\mu}(n;\mathbf{c};\mathcal{C};\mathcal{C}') = \frac{\rho_{\mu\mu}(n;\mathbf{c};\mathcal{C}') - \rho_{\mu\mu}(n;\mathbf{c};\mathcal{C})}{\rho_{\mu\mu}(n;\mathbf{c};\mathcal{C}')}. \tag{3}$$

For example in spin-valve structures $\mathcal{C}'$ and $\mathcal{C}$ refer to ''antiparallel'' and ''parallel'' alignments of the magnetizations of the magnetic slabs, and this ratio is referred to as the giant magnetoresistance (GMR) ratio. We adopt this definition of the GMR ratio, rather than the one used to report experimental results (in which the denominator is the resistivity of the parallel configuration), because the ratio given by Eq. (3) is bounded between zero and one. However, when presenting our results we will show values corresponding to both definitions of the GMR ratio; while the absolute values will of course be different for the two definitions, the conclusions drawn are usually not affected by the choice of definition. The ratio in Eq. (3) also serves as a definition for the anisotropic magnetoresistance of homogeneously disordered bulk alloys, $c_i = c, \forall i$, with uniform magnetization, $\mathbf{M}_i = \mathbf{M}, \forall i$, with $\mathcal{C}'$ and $\mathcal{C}$ referring to configurations with the magnetization pointing uniformally parallel and perpendicular to the current axis (however, in this case the ratio is usually taken with respect to an averaged resistivity).

In the present paper all calculations are based on self-consistent effective potentials and effective exchange fields as obtained previously[3] by using the fully relativistic, spin-polarized, screened Korringa-Kohn-Rostoker method together with the coherent-potential approximation for layered systems. For permalloy a fully relativistic spin-polarized calculation of the resistivity is essential in order to properly account for the spin-orbit coupling of the electron states as well as for the scattering by the disordered constituents of these binary alloys.[4,5] The surface-Brillouin-zone integrals needed in the evaluation of the electrical conductivity within the Kubo-Greenwood approach[1] were obtained by considering 1830 $\mathbf{k}_\parallel$ points in the irreducible wedge of the surface Brillouin zone. All scattering channels up to and including $l_{\max}=2$ were taken into account. In Ref. 3 we have made quite some effort to discuss the magnetic anisotropy properties in permalloy and permalloy-based spin-valve structures. Although in such spin-valve structures the orientation of the magnetization tends to be in plane, here—for ease of computation—we have chosen the magnetization to point perpendicular to the planes of atoms (i.e., the magnetization points along the z axis). With this choice the xx and yy components in the above equations are identical, hence we have taken the direction of the current (electric field) to be along the x axis so as to simulate the CIP transport geometry (with the magnetization pointing uniformally perpendicular to the current axis).

Consider the following systems:

$$\begin{aligned} &\text{(a)}\ \ \mathrm{Ni}_c\mathrm{Fe}_{1-c}(100)/(\mathrm{Ni}_c\mathrm{Fe}_{1-c})_n/\mathrm{Ni}_c\mathrm{Fe}_{1-c}(100), \\ &\text{(b)}\ \ \mathrm{Ni}_c\mathrm{Fe}_{1-c}(100)/(\mathrm{Ni}_c\mathrm{Fe}_{1-c})_n/\ \text{Vacuum}, \\ &\text{(c)}\ \ \text{Vacuum}/(\mathrm{Ni}_c\mathrm{Fe}_{1-c})_n/\text{Vacuum}. \end{aligned} \tag{4}$$

All three cases refer to the in-plane conductivity for a film with n monolayers of permalloy; what distinguishes them are the boundary conditions.[7] In case (a) we have outgoing boundary conditions on both sides as there is nothing that separates the film from the substrate it is deposited on nor from the overlayer that caps it, i.e., some electrons will leak out into the semi-infinite leads and their momentum information will be lost hence producing an additional contribution to the resistivity. In (b) we have a free surface on one side which makes it reflecting (the work function is finite so that the potential barrier is not infinitely high and there will be a slight leaking out of electrons into the vacuum that has to be taken into account). In the third case (c) we have a perfectly flat free standing film with reflecting boundary conditions on both sides. Only in (c) the calculated in-plane conductivities/resistivities for a perfectly flat film are principally independent of the film thickness n, at least for $n>12$; roughness would act like an outgoing boundary condition. However, for all three cases one obtains the so-called bulk residual resistivity $\rho^0(\mathbf{c};\mathcal{C})$ of substitutionally disordered binary alloys with respect to a particular magnetic configuration by taking the infinite-thickness limit[8]

$$\rho^0(\mathbf{c};\mathcal{C}) = \lim_{n\to\infty} \rho_{\mu\mu}(n;\mathbf{c};\mathcal{C}). \tag{5}$$

This infinite-thickness limit ($n\to\infty$) can be obtained easily since $n\rho_{\mu\mu}(n;\mathbf{c};\mathcal{C})$ becomes linear in n, if n is large enough; its slope simply refers to the extrapolated resistivity (see also the discussion of Fig. 2 in the next section). It should be noted that with the adopted orientation of the magnetization Eq. (5) refers to currents perpendicular to the orientation of the magnetization.

In addition, for computational purposes a finite imaginary part δ to the Fermi energy has to be used in the calculation of the conductivity $\sigma_{\mu\mu}(n;\mathbf{c};\mathcal{C};\epsilon_F + i\delta)$.[8] To designate resistivities calculated with finite δ we adopt the notation

$$\rho_{\mu\mu}(n;\mathbf{c};\mathcal{C};\delta) = 1/\sigma_{\mu\mu}(n;\mathbf{c};\mathcal{C};\epsilon_F + i\delta), \quad \mu \in \{x,y\}. \tag{6}$$

The actual resisitivity is arrived at by numerically taking the limit as the imaginary part goes to zero

$$\rho_{\mu\mu}(n;\mathbf{c};\mathcal{C}) = \lim_{\delta\to 0} \rho_{\mu\mu}(n;\mathbf{c};\mathcal{C};\delta). \tag{7}$$

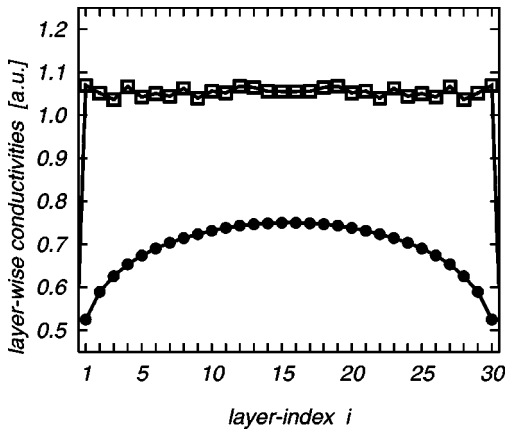

FIG. 1. Variation of the layerwise conductivities $\sigma^i_{xx}(30;0.85;\hat{\mathbf{z}};\epsilon_F+i2)$ [Eq. (8)] across the film for 30 monolayers of permalloy with a homogeneous Ni concentration of $c=0.85$ for a fixed $\delta=2$ mRyd with different boundary conditions: The values for the reflecting boundary conditions are shown as empty squares, those for the outgoing boundary conditions as full circles.

If we are interested in the bulk residual resistivity the ($\delta \rightarrow 0$) extrapolation is simplified by the fact that the slope of $n\rho_{\mu\mu}(n;\mathbf{c};\mathcal{C};\delta)$ (determined at large enough n) is itself linear in δ.

As a check on the above extrapolation procedure we used to arrive at bulk values of the resistivity from those on films of finite thickness [Eq. (5)] we have calculated in-plane resistivities (with the magnetization pointing uniformly along the z axis) for 30 monolayers of permalloy with a homogeneous Ni concentration of $c=0.85$ for a fixed $\delta=2$ mRyd with different boundary conditions: For the reflecting boundary conditions [case (c)] we find a resistivity of $\rho^{\rm ref}_{xx}(30;0.85;\hat{\mathbf{z}};2)=20.6\ \mu\Omega$ cm. A similar calculation with outgoing boundary conditions [case (a)] yields $\rho^{\rm out}_{xx}(30;0.85;\hat{\mathbf{z}};2)=31.5\ \mu\Omega$ cm which by taking $n\rightarrow\infty$ yields $\rho^{\rm out}_{xx}(\infty;0.85;\hat{\mathbf{z}};2)=20.6\ \mu\Omega$ cm; precisely the same value as found for the reflecting boundary conditions [case (c)]. This unequivocally demonstrates that the procedure outlined above is able to remove the resistivity that arises from the boundary conditions on finite structures.[7] In Fig. 1 we show as an illustration the variation of the layerwise conductivities

$$\sigma^i_{xx}(n;\mathbf{c};\mathcal{C};\epsilon_F+i\delta)=\sum_{j=1}^{n}\sigma^{ij}_{xx}(n;\mathbf{c};\mathcal{C};\epsilon_F+i\delta), \qquad (8)$$

across the film with reflecting and outgoing boundary conditions. For the outgoing boundary conditions where some electrons leak into the leads all layerwise conductivity contributions are substantially smaller than for the reflecting boundary conditions, the difference becoming progressively larger when we get closer to the outer edges of the film. When we apply reflecting boundary conditions the layerwise conductivities are practically constant with small oscillations from the boundary towards the center of the film resembling the well-known Friedel oscillations. When we take the result for $\delta=2$ mRyd corresponding to outgoing boundary conditions to $n\rightarrow\infty$ [Eq. (5)], and then numerically take the limit as $\delta\rightarrow 0$ [Eq. (7)], we find $\rho^0(0.85;\hat{\mathbf{z}})=\rho^{\rm out}_{xx}(\infty;0.85;\hat{\mathbf{z}};0)=7.1\ \mu\Omega$ cm which is the calculated resistivity for $Ni_{0.85}Fe_{0.15}$ to be compared with experiment. It should be noted, however, that the extrapolation procedures give an upper limit for the resistivity since due to computational constraints our calculations can be done only up to $n\simeq 45$ with $\delta\geqslant 2$ mRyd [i.e., the slopes of $n\rho_{\mu\mu}(n;\mathbf{c};\mathcal{C};\delta)$ might be slightly too high, and close to $\delta=0$ there might be small deviations from linearity]. Parenthetically, a similar extrapolation procedure on a film with no disorder, i.e., $c=1.0$, yields finite $\rho_{xx}(n;1.0;\mathcal{C};\delta)$ in both cases (a) and (c) for finite δ; however, the ($n\rightarrow\infty$, $\delta\rightarrow 0$) extrapolated value $\rho^{\rm out}_{xx}(\infty;1.0;\mathcal{C};0)$ for outgoing boundary conditions, as well as the ($\delta\rightarrow 0$) limit $\rho^{\rm ref}_{xx}(n;1.0;\mathcal{C};0)$ for reflecting boundary conditions, are both zero.

III. RESULTS

A. Bulk alloys

For case (b) of Eq. (4), Eq. (5) is precisely the procedure pursued in experimental studies; see Fig. 6 of McGuire and Potter[9] where the thickness dependence of the resistivity of $Ni_{0.82}Fe_{0.18}$ films is shown. It is well known that the film resistivity increases as films become thinner; the resistivity noticeable increases when the film thickness becomes much smaller than the mean free path of the conduction electrons. It is quite interesting to realize that the measured resistivity reaches its asymptotic bulk value only for film thicknesses well above 500 Å. In Fig. 2 we display the thickness dependence of our calculated $\rho^{\rm out}_{xx}(n;c;\hat{\mathbf{z}};0)$ for case (a) of Eq. (4) as a function of the number of layers n considered in the summation in Eq. (1). As can be seen, for small values of n the corresponding changes in $\rho^{\rm out}_{xx}(n;c;\hat{\mathbf{z}};0)$ are large, whereas—just as for the experimental data—for large enough n $\rho^{\rm out}_{xx}(n;c;\hat{\mathbf{z}};0)$ approaches towards its asymptotic value, i.e., the functional behavior of $n\rho^{\rm out}_{xx}(n;c;\hat{\mathbf{z}};0)$ becomes linear in n. Inspecting our ($n\rightarrow\infty$) extrapolation we find (again in accordance with experiment) that above 585 Å ($\hat{=}330$ monolayers) the deviations from the bulk residual resistivity are smaller than 1 $\mu\Omega$ cm, i.e., in order to talk about ''bulk'' in terms of resistivities one has to consider a tremendously thick film of several thousands Å. It should be noted that in order to arrive at bulk resistivities the same kind of linear extrapolation procedure to very large n [Eq. (5)] is done both with experimental data and with our calculated resistivities [Eqs. (1) and (2)].

In Fig. 3 we show our theoretical asymptotic bulk resistivities $\rho^0(c;\hat{\mathbf{z}})=\rho^{\rm out}_{xx}(\infty;c;\hat{\mathbf{z}};0)$ obtained by performing both limits ($n\rightarrow\infty$ and $\delta\rightarrow 0$) for the entire concentration range together with available low temperature (4.2 K) experimental data.[9–12] The overall trends of measured data can be obtained from an inspection of Fig. 1 of the section on Ni_cFe_{1-c} in Ref. 13 which shows the temperature dependence of the resistivity for the whole range of concentrations. From this figure one can see that by lowering the temperature the electrical resistivity becomes increasingly sensitive to the struc-

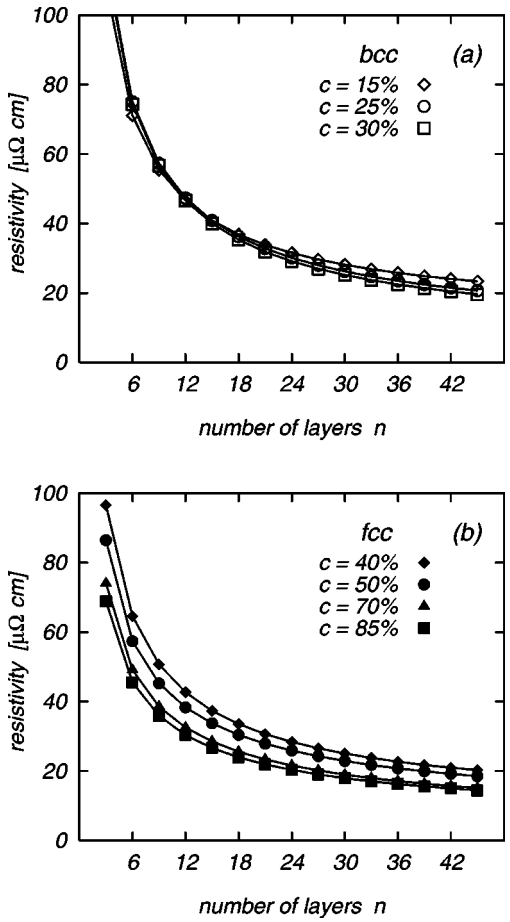

FIG. 2. Thickness dependence of the current-in-plane resistivity in bcc (a) and fcc (b) $Ni_cFe_{1-c}(100)/(Ni_cFe_{1-c})_n/Ni_cFe_{1-c}(100)$ alloys $[\rho_{xx}^{\rm out}(n;c;\hat{\mathbf{z}};0)]$. The Ni concentration in % is indicated explicitly; n denotes the number of layers considered in the summation in Eq. (1).

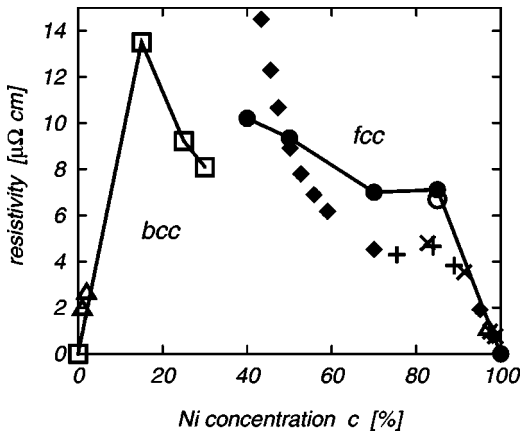

FIG. 3. Concentration dependence of the current-in-plane resistivity of ''bulk'' Ni_cFe_{1-c} alloys calculated as the infinite-thickness limit of $Ni_cFe_{1-c}(100)/(Ni_cFe_{1-c})_{n\to\infty}/Ni_cFe_{1-c}(100)[\rho^0(c;\hat{\mathbf{z}})=\rho_{xx}^{\rm out}(\infty;c;\hat{\mathbf{z}};0)]$. The results for the bcc α phase are shown as empty squares, for the fcc γ phase as full circles, and the open circle at $c=85\%$ refers to a calculation with $l_{\max}=3$. Low temperature (4.2 K) experimental values are displayed by crosses (Ref. 9), diamonds (Ref. 10), pluses (Ref. 11), and open triangles (Ref. 12).

tural phase transition from bcc to fcc; at the temperature of liquid nitrogen (-195 C, the lowest isothermal curve displayed) in the Fe-rich bcc α phase the resistivity reaches a maximum at about 15% of Ni and then slowly decreases up to 30% of Ni, whereas in the Ni-rich fcc γ phase the resistivity starts to grow below 50% of Ni and seems to diverge near the critical concentration for the structural phase transition. This anomalous increase in resistivities and a large departure from Nordheim's law was also found by low temperature measurements.[10] In the -195 C curve we also discern a weak shoulder at about 85% Ni; this feature is well resolved in the low temperature (4.2 K) experimental data.[9–11] As can be seen from Fig. 3 our theoretical values reproduce quite well the vicinity of the rather complicated martensitic[14] structural phase transition from bcc to fcc at about 35% of Ni. There is indeed a maximum in the bcc phase at about 15% of Ni; the onset of the phase transition is clearly visible. Also—just as the experimental data—in the fcc phase the theoretical values show a kind of shoulder at about 85% of Ni.

For this concentration ($c=0.85$) we performed an additional calculation using a maximum angular momentum quantum number $l_{\max}=3$ (see also Ref. 15). As can be seen from Fig. 3, the difference between the $l_{\max}=3$ and the $l_{\max}=2$ (that is used in all other calculations) results is rather small; however the trend for the inclusion of higher scattering channels is to lower (slightly) the resistivity.

Although the theoretical resistivities agree rather well with the experimental ones, the difference at a particular concentration being of the order of 3 $\mu\Omega$ cm, it seems appropriate to comment on the putative sources of the difference. First of all, in the present use of the Kubo-Greenwood equation for layered systems no vertex corrections arising from the configurational average of the product of two Green's functions are included (see also the discussion in Ref. 1). In another calculation[4,5] of the resistivity of bulk Ni_cFe_{1-c} the vertex corrections were calculated and found to be quite small over the entire range of concentrations,[16] i.e., no larger than the differences between the $l_{\max}=2$ and $l_{\max}=3$ results at $c=0.85$ in Fig. 3. Second, the single site approximation to the coherent-potential approximation is used to describe the electronic structure of substitutional alloys. This in turn implies that short range order or concentration fluctuations are excluded. Both the inclusion of vertex corrections and the inclusion of short range order will reduce the present theoretical resistivity values. Furthermore, in magnetic alloys magnetic ordering or clustering can occur; as it implies some ordering, which we have not taken into account, it will again (slightly) lower the resistivity.

In two previous theoretical papers[4,5] the validity of the so-called two-current model for transport in ferromagnetic systems with strong spin-dependent disorder was tested; the resistivity and the anisotropic magnetoresistance for Ni_cFe_{1-c} bulk alloys was calculated by solving the Kubo-Greenwood equation using a spin-polarized, relativistic version of the Korringa-Kohn-Rostoker method together with the coherent-potential approximation. As these calculations were done on a fcc lattice for the whole concentration range

their results are not applicable to the Fe-rich bcc alloys. Nonetheless a very weak shoulder at about 80% Ni can be discerned from their Fig. 4 (Ref. 4)—in agreement with the experimental data and our present calculation; see Fig. 3. However, the resistivities they find for 80% Ni, $\rho \simeq 1.8\ \mu\Omega$ cm, as well as the maximum at about 40% Ni, $\rho \simeq 3.2\ \mu\Omega$ cm, are too low by about a factor of 2 as compared to available experimental data.

It should be noted that a nonrelativistic calculation[6] of the resistivity in the fcc phase of Ni_cFe_{1-c} bulk alloys yielded much too low values and failed to describe the above mentioned shoulder at about 80% Ni. Since no technical details of the applied approach were given and since the effect of spin-orbit coupling was only roughly estimated, no further comparison to the present fully relativistic calculations can be made.

B. Spin-valve structures

The main purpose of our study has been to show how well resistivities for disordered magnetic systems with only two-dimensional translational symmetry (films) can be described, and to confirm that by taking the appropriate limit we derive the bulk resistivities from those calculated for films. Since a large number of spin-valve structures that are used in applications, e.g., the read heads of hard disk drives, contain permalloy layers, we conclude with some results on their transport properties. Including permalloy layers into a multilayer system the electronic structure and the magnetic properties are considerably more complicated than for bulk permalloy; specifically they are sensitive to the thickness and Ni concentration c of the permalloy layers, and to the constituency of the neighboring layers. Therefore for concreteness we focus on a permalloy-based system that has been studied, e.g., Si substrate/Cu contacts(1500 Å)/Ni_cFe_{1-c}(100 Å)/Co(6 Å)/Cu(9 Å)/Co(6 Å)/Ni_cFe_{1-c}(5 Å)/NiO(250 Å),[17] and we replace it with the reference system $Ni_cFe_{1-c}(100)/(Ni_cFe_{1-c})_{12}Co_4Cu_nCo_4(Ni_cFe_{1-c})_3$/Vacuum. In all cases shown a fcc(100) stacking was chosen, the lattice spacing refers to that of the corresponding fcc bulk Ni_cFe_{1-c} system. In this transcription the rather thick permalloy layer of about 100 Å ($\hat{=}56$ monolayers) is considered as a substrate, the insulating NiO layer is replaced by a free surface (vacuum), and all other thicknesses are expressed (in monolayers) as close as possible to the measured structure. The 12 layers of Ni_cFe_{1-c} are deliberately chosen so as to guarantee a smooth matching to the substrate via a self-consistent calculation; this in turn would also allow us to change the left boundary condition such that in principle a system of the type Vacuum/$(Ni_cFe_{1-c})_{56}Co_4Cu_nCo_4(Ni_cFe_{1-c})_3$/Vacuum could be described by assuming that the layers in the very interior of the thick Ni_cFe_{1-c} layer exhibit bulk-like properties.

We have considered two series: in the first the Cu-spacer thickness is confined to $n=5$ and we vary the Ni concentration c while maintaining an fcc lattice throughout; in the second we set $c=0.85$ and vary the number of Cu-spacer layers n. While the structure of Ni_cFe_{1-c} bulk alloys is bcc for $c<35\%$ when there are relatively thin layers in a fcc multilayered structure it is appropriate to maintain the fcc lattice structure even for the Fe-rich alloys. In the parallel configuration of the spin valve the magnetizations of all permalloy and Co layers are aligned uniformly perpendicular to the plane of the layers; in the antiparallel configuration they are still normal to the layers but the magnetizations of the two magnetic slabs (separated by the Cu spacer) point in opposite directions to one another. The conductivity is evaluated at a finite imaginary part to the Fermi energy, $\delta = 2$ mRyd; this is necessary for otherwise the calculations would take an inordinate time. In principle, in order to obtain the resistivity we have to take the limit as $\delta \to 0$ [see Eq. (7)]. However, it is virtually impossible for technical reasons to do this up till now for a whole series of spin-valve structures; therefore we do not show the resistivities we calculated for finite δ. But with the assumption that both resistivities for the parallel and the antiparallel configuration of the spin valve scale uniformly with δ, and therefore cancel out in the ratio R [Eq. (3)], we have used them to estimate the CIP-MR

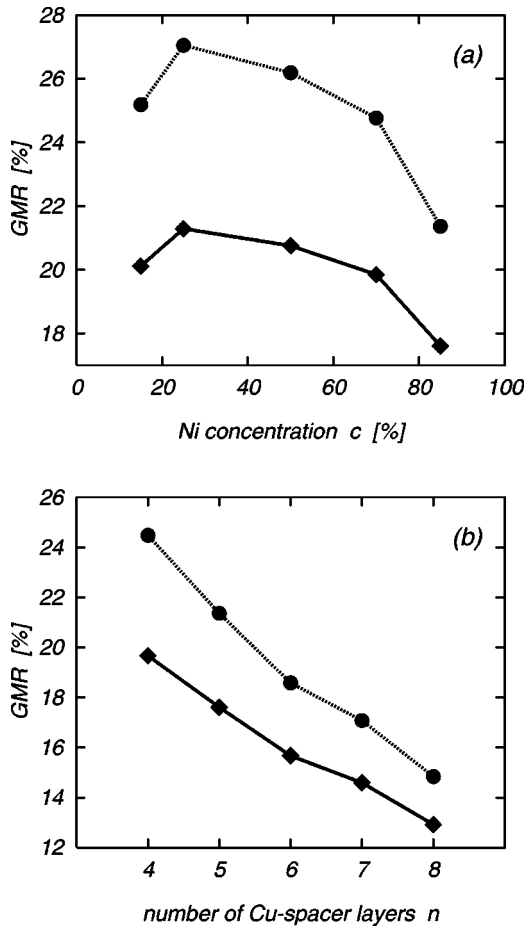

FIG. 4. Current-in-plane magnetoresistance for permalloy-based spin valves: (a) Concentration dependence for fcc-based $Ni_cFe_{1-c}(100)/(Ni_cFe_{1-c})_{12}Co_4Cu_5Co_4(Ni_cFe_{1-c})_3$/Vacuum systems. (b) Dependence on the number of Cu-spacer layers n in fcc-based $Ni_{0.85}Fe_{0.15}(100)/(Ni_{0.85}Fe_{0.15})_{12}Co_4Cu_nCo_4(Ni_{0.85}Fe_{0.15})_3$/Vacuum. The CIP-MR ratio defined by Eq. (3) is shown as diamonds, its alternative definition (i.e., the ratio taken with respect to the parallel configuration) as circles.

ratios that one can expect from these spin-valve structures. As we have chosen the orientation of the magnetization to be perpendicular to the current our calculations should be compared only to measurements for the current in the plane of the layers perpendicular to the magnetization, otherwise anisotropic magnetoresistance contributions of permalloy enter. Since we found that the band energy effects to the magnetic anisotropy energy in permalloy-related spin valves are quite small, we can anticipate that the GMR will not change much when one rotates the magnetization in the plane of the layers.

In Fig. 4(a) we show the variation of the calculated CIP-MR ratio of the reference system with the Ni concentration c for the fixed Cu-spacer thickness $n=5$. As can be seen the CIP-MR varies only very little [17.5–21.5 % and 21.5–27.0 % for the two definitions of the GMR ratio; see also the comment after Eq. (3)] over the whole range of concentrations considered. In Fig. 4(b) we show the variation of the CIP-MR ratio for the reference system corresponding to $c=0.85$ with respect to the number of Cu-spacer layers n. By doubling the number of Cu-spacer layers, i.e., by going from $n=4$ to $n=8$, the CIP-MR is reduced by almost a factor of two (again independent of the choice of definition of the GMR). This dramatic decrease can be understood in terms of a simple model: since on increasing the thickness of the nonmagnetic spacer layer t_{nm} the CIP-MR decreases as $(1/t_{\mathrm{nm}})\exp(-t_{\mathrm{nm}}/\lambda_{\mathrm{nm}})$,[2] where λ_{nm} is the mean free path of the conduction electrons in the nonmagnetic spacer layer, the ratio $R_{xx}(t_{\mathrm{nm}})/R_{xx}(2t_{\mathrm{nm}})\approx 2$ for $t_{\mathrm{nm}}\ll\lambda_{\mathrm{nm}}$ (which is a necessary condition to find at all a CIP-MR and certainly valid for our t_{nm} varying between 7.1 Å and 14.2 Å). Our findings seem to be confirmed by experiments made on similar systems[18] albeit at room temperature, while our calculated values are for $T=0$ K. Depending on the actual thicknesses of the bottom and top Ni_cFe_{1-c} layers, of the Co slabs and of the Cu spacer, and the pinning and capping layers used, the experimental CIP-MR ratios in permalloy-related spin-valve systems have been found to be in the range between 10 and 20%. Figure 4 shows that this is about the range that our theoretical calculations predict when we use the resistivities calculated with finite δ, and when we make the assumption that for both the parallel and the antiparallel configurations of the spin valve the resistivity scales uniformly with δ and therefore cancels out in the CIP-MR ratio R.

IV. SUMMARY

By using our fully relativistic, spin-polarized, screened Korringa-Kohn-Rostoker method together with the coherent-potential approximation for layered systems we have calculated the resistivity across the entire Ni_cFe_{1-c} (permalloy) series of bulk alloys within the Kubo-Greenwood approach. We are able to reproduce the overall variation of the resistivity as a function of the Ni concentration; in particular we reproduce the discontinuity in the vicinity of the structural change from bcc to fcc. Also we obtain very reasonable absolute values for the resistivities. We have also estimated the CIP-MR ratios for permalloy-based spin-valve structures and within the limits of our current calculation find trends that are in reasonably good agreement with those measured on prototypical spin valves; there is of course the caveat that most of the data on spin valves is quoted at room temperature while our results are for $T=0$ K. It should be stressed that our results are based on *ab initio* calculations with no adjustable parameters. Viewed in this light the calculated resistivities and GMR ratios are noteworthy.

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