

Race Track Memories Seen from an *Ab Initio* Point of View

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In using the fully relativistic versions of the screened Korringa-Kohn-Rostoker method and of the Kubo-Greenwood equation equilibrium domain wall widths and corresponding domain wall resistivities are calculated for $\text{Co}_c\text{Fe}_{1-c}$ and $\text{Co}_c\text{Ni}_{1-c}$ making use of a multiscale approach. It is found that in $\text{Co}_c\text{Fe}_{1-c}$ the domain wall width becomes rather large at about $c = 0.4$, but does not show an obvious singularity in the vicinity of the bcc to fcc phase transition. In $\text{Co}_c\text{Ni}_{1-c}$ the domain wall width varies much less in size with respect to the concentration. In particular, it is demonstrated that as compared to the homogeneous infinite systems the anisotropic magnetoresistance is reduced in the presence of a domain wall. This reduction is rather big for $\text{Co}_c\text{Ni}_{1-c}$, namely, about 6%, while for $\text{Co}_c\text{Fe}_{1-c}$ it is only of the order of 1%–2%. The results clearly indicate that $\text{Co}_c\text{Ni}_{1-c}$ might be a useful candidate for race track memories.

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One of the most fascinating new ideas in the field of spintronics is the concept of race track memories [1–3], which is based on the experimental finding that in a given length of a nanowire the size of the anisotropic magnetoresistance (AMR) changes whether a domain wall is present or not. Since domain walls can be moved in and out such a predefined region by applying an electric field [4], it was proposed to use this effect for a new, all-solid-state archival storage with about the same density of magnetic disks, however, with no moving parts at all. Very recently it was shown that already very short pulses of the order of a few picoseconds of an electric field [5,6] are sufficient to cause a domain wall to move. Quite clearly there are still quite a few experimental difficulties to resolve such as, e.g., the problem of depinning [7–9]; however, once all obstacles are removed, it seems that such a device will depend only on the speed by which changes in the AMR can be recorded. Surprisingly enough, up-to-now all (reported) experimental investigations were confined to permalloy with a nickel concentration near 85%.

From a theoretical standpoint of view two, rather very different aspects of race track memories have to be addressed, namely, (i) what causes a domain wall to move when an electric field is applied, and (ii) can the experimental evidence be confirmed that the AMR is *reduced* [7] in the presence of a domain wall, and if so, are there other magnetic materials than permalloy equally suitable for the envisaged purpose? With respect to the first question only very recently first attempt were made to describe the interaction of an external (time-dependent) electromagnetic field with a magnetic system by using the time-dependent Dirac equation [10], a concept, which in turn offers the possibility to define all occurring torque terms rigorously. The second question, which is addressed in here, not only requires to determine equilibrium domain wall widths, but also to calculate respective domain wall resistivities and the AMR in the absence of domains walls for statistically disordered systems.

As is well known, two of the three possible binary substitutional alloys of magnetic 3d-metals, namely $\text{Fe}_c\text{Ni}_{1-c}$ and $\text{Co}_c\text{Fe}_{1-c}$, show phase transitions from bcc to fcc and are therefore only useful in certain concentration regimes. $\text{Co}_c\text{Ni}_{1-c}$, however, with the exception of very diluted alloys remains fcc over the whole concentration range. In here the systems $\text{Co}_c\text{Fe}_{1-c}$ and $\text{Co}_c\text{Ni}_{1-c}$ are considered in response to the second question raised above.

Suppose L denotes the width of a domain wall, C its magnetic configuration, c the concentration and $A_0(c)$ the unit area in a magnetic substitutional binary alloy A_cB_{1-c} then the domain wall formation energy can be written as [11,12]

$$E(L; C, c) = A_0(c) \left(\frac{\alpha(C, c)}{L} + \beta(C, c)L \right), \quad (1)$$

where the constants $\alpha(C, c)$ and $\beta(C, c)$ correspond to the exchange and anisotropy energy, respectively. Given the values of $E(L; C, c)$ at two points L_1 and L_2 , the constants $\alpha(C, c)$ and $\beta(C, c)$ can be evaluated and therefore also the minimum of $E(L; C, c)$ and the corresponding equilibrium domain wall width L_0 .

Suppose now that C_0 and C_1 denote the following magnetic reference configurations,

$$C_0 = \{\vec{n}_l = \vec{x}, \vec{n}_i = \vec{x}, \vec{n}_r = \vec{x}, i = 1, L\}, \quad (2)$$

$$C_1 = \{\vec{n}_l = \vec{z}, \vec{n}_i = \vec{z}, \vec{n}_r = \vec{z}, i = 1, L\}, \quad (3)$$

where \vec{n}_l and \vec{n}_r denote the orientations of the magnetization in the “left” and the “right” domain, the \vec{n}_i those in the atomic planes forming the wall, \vec{x} is parallel to the in-plane x axis, and \vec{z} is parallel to the surface normal. Suppose further a magnetic configuration C_d such that within the atomic layers forming the domain wall the orientation of the magnetization in the individual planes changes continuously from \vec{x} to $-\vec{x}$

$$C_d = \{\vec{n}_l = \vec{x}, \vec{n}_i, \vec{n}_r = -\vec{x}, i = 1, L\}, \quad (4)$$

$\vec{n}_i = D(\Phi_i)\vec{x}$, $\Phi_i = 180i/L$, $i = 1, \dots, L$, $D(\Phi_i)$ being a rotation by an angle Φ_i around the surface normal. For a particular value of L the domain wall formation energy $E(L; C_d, c)$ can now be evaluated as the difference in the grand canonical potentials between two configurations, e.g., C_d and C_0 ,

$$E(L; C_d, c) = \int_{E_b}^{E_F} [n(L; C_d, c; \epsilon) - n(L; C_0, c, \epsilon)](\epsilon - E_F) d\epsilon, \quad (5)$$

where $n(L; C_i, c, \epsilon)$ is the density of states (in L unit cells) corresponding to a particular configuration C_i , and E_b and E_F denote the valence band bottom and the Fermi energy, respectively. It should be noted that by adding L_l and/or L_r layers from the left or right domain, the domain wall formation energy remains unchanged, i.e., $E(L + L_l + L_r; C_d, c) = E(L; C_d, c)$.

In principle for a particular magnetic configuration C_i the current perpendicular to the planes of atoms (CPP) defined over a certain length L is given by [13]

$$\rho_{\text{CPP}}(L; C_i, c) = \frac{1}{L} \iint_{-\infty}^{\infty} \rho(z, z'; C_i, c) dz dz', \quad (6)$$

and the corresponding sheet resistance by

$$r(L; C_i, c) = L \rho_{\text{CPP}}(L; C_i, c). \quad (7)$$

For large enough L the resistivity $\rho_{\text{CPP}}(L; C_i, c)$ can be obtained from the zz component of the conductivity tensor, $\rho_{zz}(L; C_i, c)$,

$$\rho_{\text{CPP}}(L; C_i, c) \sim \rho_{zz}(L; C_i, c) = \sigma_{zz}^{-1}(L; C_i, c). \quad (8)$$

As it is virtually impossible to calculate the conductivity tensor by means of *ab initio* methods for very large L one can make use of the fact that $r(L; C_i, c)$ is linear in L ,

$$r(L; C_i, c) = L \rho_{zz}(L; C_i, c) = a(C_i, c) + b(C_i, c)L. \quad (9)$$

If used in practical terms this linear form has to yield the below limiting properties

$$0 < c < 1: \lim_{L \rightarrow \infty} \rho_{zz}(L; C_d, c) = b(C_d, c) = \rho_{zz}(C_0, c), \quad (10)$$

$$c = 0, 1: \lim_{L \rightarrow \infty} \rho_{zz}(L; C_d, c) = \rho_{zz}(C_0, c) = 0, \quad (11)$$

where $\rho_{zz}(C_0, c)$, $0 < c < 1$, is the zz component of the residual (bulk) resistivity corresponding to configuration C_0 ; see Eq. (2). As is well-known for pure systems ($c = 0, 1$) the constant $b(C, c)$ has to be exactly zero. Equation (11) can therefore be used to check the accuracy of the applied numerical procedure, in particular, since $\rho_{zz}(L; C, c)$ is evaluated by means of an analytical continuation of resistivities defined for complex Fermi energies [14].

Clearly enough the “standard” expression for the anisotropic magnetoresistance [15] for bulk cubic systems, $c \neq 0, 1$, no longer makes sense in the presence of domain

walls. However, for $L_0 \gg 0$ one can define a similar ratio,

$$\text{AMR}(L_0; C_i, c) = \frac{\rho_{zz}(L_0; C_1, c) - \rho_{zz}(L_0; C_i, c)}{\rho_{zz}(L_0; C_1, c)}, \quad (12)$$

$C_i = C_0, C_d$, where L_0 now refers to the equilibrium domain wall width. Similarly, in the absence of domain walls use can be made of Eq. (10), i.e.,

$$\text{AMR}(c) = [\rho_{zz}(C_1, c) - \rho_{zz}(C_0, c)]/\rho_{zz}(C_1, c). \quad (13)$$

Finally, a difference in these anisotropic magnetoresistances can be evaluated,

$$\Delta_{\text{AMR}} = \text{AMR}(L_0; C_i, c) - \text{AMR}(c), \quad (14)$$

which indicates how much the AMR is changed due to the presence of a domain wall.

All *ab initio* calculations were performed using the spin-polarized relativistic screened Korringa-Kohn-Rostoker (SPR-KKR) method in the atomic sphere approximation (ASA), for details see Ref. [16], and the local density functional parametrization given in Ref. [17]. For each concentration of $\text{Co}_c\text{Fe}_{1-c}$ and $\text{Co}_c\text{Ni}_{1-c}$ the effective potentials and exchange fields were calculated self-consistently at the corresponding experimental lattice spacing by means of the inhomogeneous coherent potential approximation [16] using 45 k points in irreducible part of the surface Brillouin zone (ISBZ) placing the orientation of the magnetization uniformly along \vec{x} (configuration C_0). Using these potentials and exchange fields the grand potentials $E(L; C_d, c)$ in Eq. (5) were evaluated by means of a contour integration along a semicircle using a 16 point Gaussian-quadrature and 1830 k points per ISBZ. The electric transport properties were evaluated at complex Fermi energies by means of the fully relativistic Kubo equation [14] using also 1830 k points per ISBZ and then analytically continued to the real axis. It turns out that in using Eqs. (8)–(11) the inherent numerical errors are rather very small. For bcc Fe $\rho_{zz}(C_0, c = 1)$ is predicted to be $-0.063 [\mu\Omega \cdot \text{cm}]$ instead of being exactly zero, for fcc Co the remaining error amounts to $0.060 [\mu\Omega \cdot \text{cm}]$.

In Fig. 1 the exchange and anisotropy energies α and β for $\text{Co}_c\text{Fe}_{1-c}$ and $\text{Co}_c\text{Ni}_{1-c}$, see Eq. (1), are displayed versus the Co concentration together with the corresponding equilibrium domain wall width L_0 . While for $\text{Co}_c\text{Ni}_{1-c}$ α , β and L_0 vary fairly smoothly with c , in $\text{Co}_c\text{Fe}_{1-c}$ both α and β show a break in the vicinity of the phase transition: they change from higher values in the bcc regime to lower values in the fcc regime. It is interesting to note that although there is this discontinuity for α and β across the regime of the phase transition, by continuing “artificially” the bcc regime to $c = 0.8$ no obvious jump in L_0 occurs at that concentration. Since the structural phase transition extends over about 20% in concentration and since the α and β are defined strictly only for either the bcc or the fcc regime, unfortunately nothing can be said about how they would change in the concentration range of the

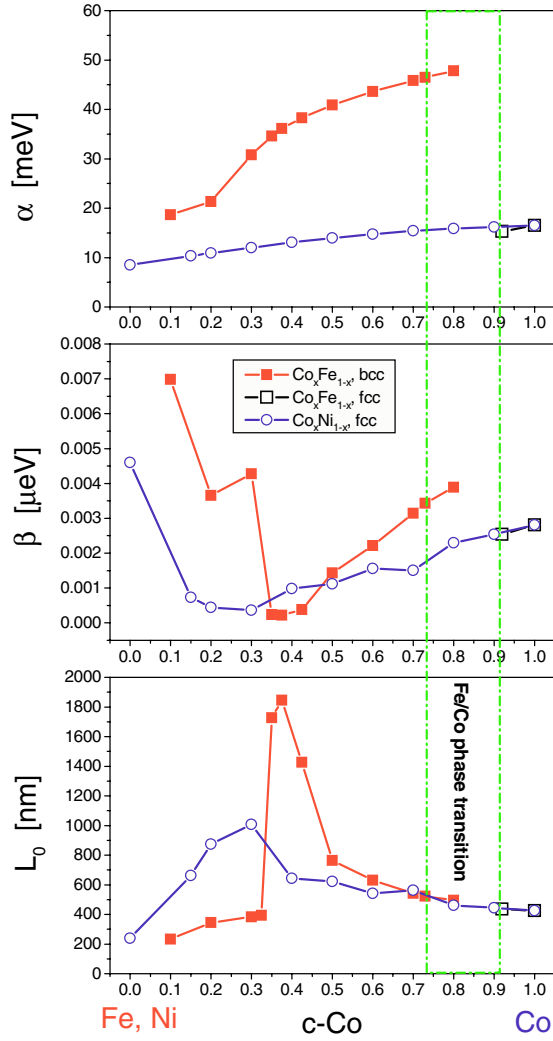


FIG. 1 (color online). Fitting parameters α and β , see Eq. (1), and equilibrium domain wall width [nm] in $\text{Co}_c\text{Fe}_{1-c}$ and $\text{Co}_c\text{Ni}_{1-c}$ with respect to the Co concentration.

phase transition. Furthermore, since for $\text{Co}_c\text{Fe}_{1-c}$ β reaches a minimum while α increases continuously with c , there is a peak in L_0 near $c \sim 0.4$. This minimum in β looks like as if the system attempts to head for a structural phase transition. In $\text{Ni}_c\text{Fe}_{1-c}$, for example, both α and β tend to zero right before the structural phase transition from fcc to bcc [12]. In $\text{Co}_c\text{Fe}_{1-c}$ the actual value of the minimum in β might be overrated by the lack of short range order, which in the so-called single site coherent potential approximation [16] is not included. However, since coming from lower and from higher Co concentrations β has different slopes, similarly to the case of $\text{Co}_c\text{Ni}_{1-c}$ a minimum must occur.

In Figs. 2 and 3 the resistivities $\rho(C_0, c)$ and $\rho(C_1, c)$, namely, the so-called bulk residual resistivities, see Eq. (10), are displayed versus the Co concentration together with $\rho(L_0; C_0, c)$, $\rho(L_0; C_1, c)$ and $\rho(L_0; C_d, c)$. In the case of $\text{Co}_c\text{Ni}_{1-c}$ also the experimental room tempera-

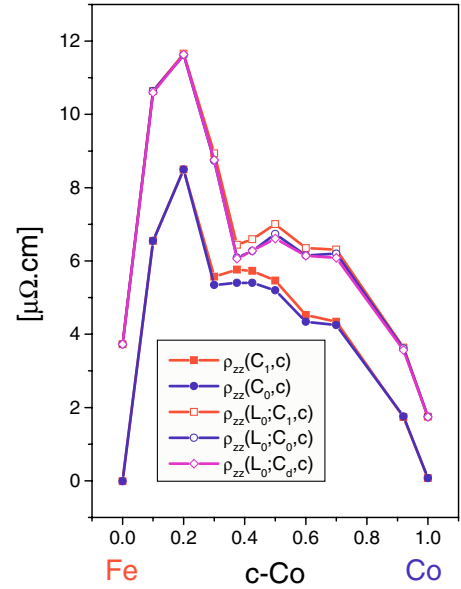


FIG. 2 (color online). Domain wall resistivities $\rho_{zz}(L_0; C_i, c)$ and bulk resistivities $\rho_{zz}(C_i, c)$, for $\text{Co}_c\text{Fe}_{1-c}$. The various entries are denoted explicitly.

ture values of Ref. [18] are shown. Note that for illustrative purposes these values were shifted uniformly by $-5 [\mu\Omega \cdot \text{cm}]$ such that for pure Co the experimental value is zero. As can be seen from Fig. 3 for $\text{Co}_c\text{Ni}_{1-c}$ the experimental and the theoretically calculated “bulk” resistivities vary in a similar manner with respect to the Co concentration. There is a peak at about $c = 0.15$, for higher Co concentrations the resistivities fall off continuously. For both

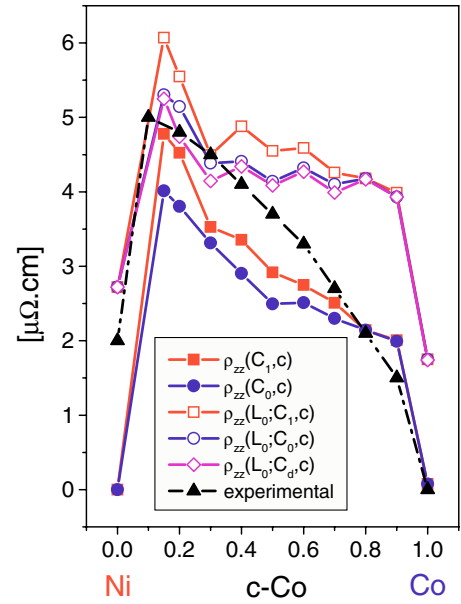


FIG. 3 (color online). Domain wall resistivities $\rho_{zz}(L_0; C_i, c)$ and bulk resistivities $\rho_{zz}(C_i, c)$, for $\text{Co}_c\text{Ni}_{1-c}$. The various entries are denoted explicitly, the experimental values [18] at 273° K, are shifted uniformly by $-5 [\mu\Omega \cdot \text{cm}]$.

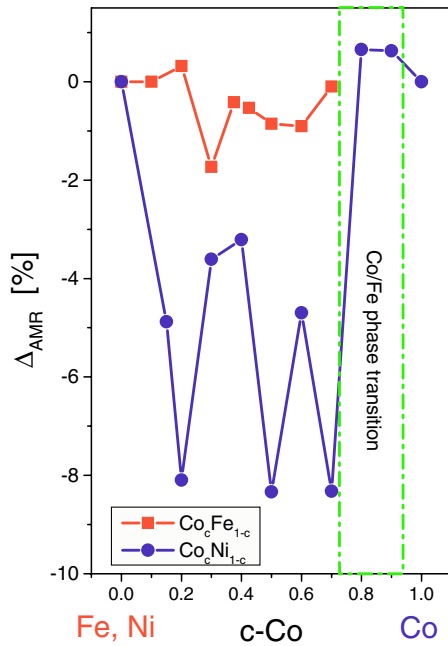


FIG. 4 (color online). Difference in the AMR due to the presence of a domain wall, see Eq. (14).

systems $\rho(L_0; C_0, c)$ and $\rho(L_0; C_d, c)$ are very similar in value, since the so-called in-plane anisotropy is very small.

Finally Fig. 4 comprises the main result of this study, namely, the difference in the anisotropic magnetoresistance with respect to the presence and the absence of a domain wall; see Eqs. (12)–(14). From this figure one can immediately see that the system $\text{Co}_c\text{Fe}_{1-c}$ obviously is not suitable for technological purposes, while the results for $\text{Co}_c\text{Ni}_{1-c}$ suggest that for $0.15 \leq c \leq 0.75$ on the average a reduction of the AMR amounting to about 6% can be expected.

In order to understand these results properly consider a segment of a “wire” consisting of $L \geq L_0$ atomic layers, namely, exactly of that length that corresponds to the definition in Eq. (6), i.e., of that length that separates the (prefixed) contacts. If there is no domain wall present, the AMR to be recorded refers to the bulk value. If, however, a domain wall (of length L_0) occurs within these L atomic layers, the corresponding AMR is different, namely, smaller than the bulk value. Moving therefore the domain wall in and out the predefined segment by applying an electric current, the difference in the AMR, Δ_{AMR} , jumps by about 1% in the case of $\text{Co}_c\text{Fe}_{1-c}$ and about 6% for $\text{Co}_c\text{Ni}_{1-c}$. In permalloy, $\text{Ni}_c\text{Fe}_{1-c}$ the reduction of the AMR is confined to $0.6 \leq c < 1$. Near 80% Ni, where experimental studies up to now were performed, theoretical investigations [19] showed that this reduction amounts to about 16%. Reduction of the AMR as should be recalled

is exactly the underlying idea for a race track memory. Clearly enough the present results do not contain an interaction with the applied electric field beyond the linear response regime and can therefore not describe the actual motion of domain walls. This, however, is a completely different aspect of generating race track memories, which has to be dealt with separately using different theoretical means [10].

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