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 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 might be a useful candidate for race track memories.

As is well known, two of the three possible binary substitutional alloys of magnetic 3d-metals, namely Fe1−cNi−c and Co1−cFe−c, show phase transitions from bcc to fcc and are therefore only useful in certain concentration ranges. Co1−cNi−c, however, with the exception of very diluted alloys remains fcc over the whole concentration range. In here the systems Co1−cFe−c and Co1−cNi−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 A0(c) the unit area in a magnetic substitutional binary alloy A1−cBc then the domain wall formation energy can be written as

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

(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,

$$C_0 = \{ \tilde{n}_i = \tilde{x}, \tilde{n}_i = \tilde{x}, \tilde{n}_r = \tilde{x}, i = 1, L \},$$

(2)

$$C_1 = \{ \tilde{n}_i = \tilde{z}, \tilde{n}_i = \tilde{z}, \tilde{n}_r = \tilde{z}, i = 1, L \},$$

(3)

where $\tilde{n}_i$ and $\tilde{n}_r$ denote the orientations of the magnetization in the “left” and the “right” domain, those in the atomic planes forming the wall, $\tilde{x}$ is parallel to the in-plane x axis, and $\tilde{z}$ 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 $\tilde{x}$ to $-\tilde{x}$

$$C_d = \{ \tilde{n}_i = \tilde{x}, \tilde{n}_r = -\tilde{x}, i = 1, L \}.$$
evaluated by means of an analytical continuation of resistive magnetoresistance \[15\] for bulk cubic systems, can make use of the fact that

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

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

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

\[
\rho_{\text{CPP}}(L; C_d; c) = \frac{1}{L} \int_{-\infty}^{\infty} \rho(z, z'; C_d; c) dz dz',
\]

and the corresponding sheet resistance by

\[
r(L; C_d; c) = L \rho_{\text{CPP}}(L; C_d; c).
\]

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

\[
\rho_{\text{CPP}}(L; C_d; c) = \rho_{zz}(L; C_d; c) = \sigma_{zz}^{-1}(L; C_d; c).
\]

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

\[
r(L; C_d; c) = L \rho_{zz}(L; C_d; c) = a(C_d; c) + b(C_d; c)L.
\]

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

\[
0 < c < 1: \lim_{L \to \infty} \rho_{zz}(L; C_d; c) = b(C_d; c) = \rho_{zz}(C_0; c),
\]

\[
c = 0, 1: \lim_{L \to \infty} \rho_{zz}(L; C_d; c) = \rho_{zz}(C_0; c) = 0,
\]

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,

\[
\Delta_{\text{AMR}} = \Delta_{\text{AMR}}(L_0; C_d; c) = \frac{\rho_{zz}(L_0; C_1; c) - \rho_{zz}(L_0; C_0; c)}{\rho_{zz}(L_0; C_1; c)},
\]

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.,

\[
\Delta_{\text{AMR}}(c) = \frac{\rho_{zz}(C_1; c) - \rho_{zz}(C_0; c)}{\rho_{zz}(C_1; c)}.
\]

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

\[
\Delta_{\text{AMR}} = \Delta_{\text{AMR}}(L_0; C_d; c) - \Delta_{\text{AMR}}(c),
\]

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

All \textit{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 Co, Fe\(_{1-c}\) and Co, Ni\(_{1-c}\) the 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 \(\hat{x}\) (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 \(\alpha\) and \(\beta\) for Co\(_{0.75}\), Fe\(_{0.25}\) and Co\(_{0.75}\), Ni\(_{0.25}\), see Eq. (1), are displayed versus the Co concentration together with the corresponding equilibrium domain wall width \(L_0\). While for Co\(_{0.75}\), Ni\(_{0.25}\) \(\alpha, \beta\) and \(L_0\) vary fairly smoothly with \(c\), in Co\(_{0.75}\), Fe\(_{0.25}\) both \(\alpha\) and \(\beta\) 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 \(\alpha\) and \(\beta\) 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 \(\alpha\) and \(\beta\) 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
phase transition. Furthermore, since for Co$_{c}$Fe$_{1-c}$ $\beta$ reaches a minimum while $\alpha$ increases continuously with $c$, there is a peak in $L_0$ near $c \sim 0.4$. This minimum in $\beta$ looks like as if the system attempts to head for a structural phase transition. In Ni$_{c}$Fe$_{1-c}$, for example, both $\alpha$ and $\beta$ tend to zero right before the structural phase transition from fcc to bcc [12]. In Co$_{c}$Fe$_{1-c}$ the actual value of the minimum in $\beta$ 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 $\beta$ has different slopes, similarly to the case of Co$_{c}$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 $\rho(L_0;C_{d_{c}}, c)$. In the case of Co$_{c}$Ni$_{1-c}$ also the experimental room temperature 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 Co$_{c}$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
systems $\rho(L_0; C_0, c)$ and $\rho(L_0; C_a, c)$ 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 CoFe$_{1-c}$ obviously is not suitable for technological purposes, while the results for Co$_x$Ni$_{1-x}$ 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, $\Delta_{AMR}$, jumps by about 1% in the case of Co$_x$Fe$_{1-c}$ and about 6% for Co$_x$Ni$_{1-x}$. In permalloy, Ni$_c$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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