

Concentrational restrictions for race track memories based on permalloy

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One of the most fascinating new ideas in the field of spintronics is the concept of race track memories,[1, 2, 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.[9, 7, 8] 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%. In this contribution it is shown that in permalloy, the most favorite system in respective experimental studies, the AMR is **reduced** [7] in the presence of a domain wall only in a rather narrow regime of concentrations implying that this is the only regime in which "race tracking" can only be realized.

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 [10, 11]

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

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,

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

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

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 $-\vec{x}$

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

$\vec{n}_i = D(\Phi_i)\vec{x}$, $\Phi_i = 180i/L$, $i = 1, \dots, L$, $D(\Phi_i)$ being a rotation by an angle Φ_i around the surface normal.

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 [12]

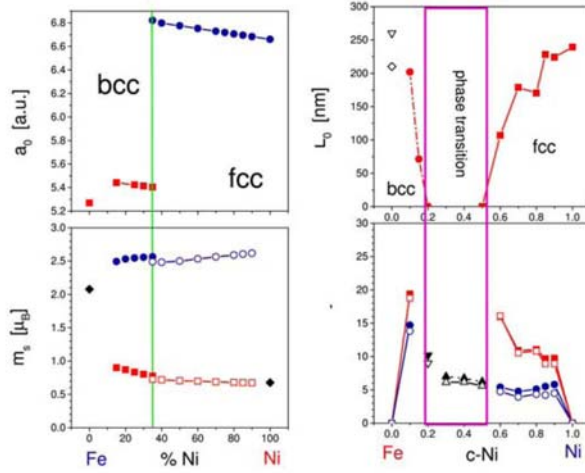


Figure 1: Left: Experimental lattice constants and spin-only magnetic moments in $\text{Ni}_c\text{Fe}_{1-c}$. Right: Top: Equilibrium domain wall width [nm], Ref. [11], bottom: domain wall resistivities $\rho_{zz}(L_0; C_i, c)$ and "bulk" resistivities $\rho_{zz}(C_i, c)$, $C_i = C_1, C_d$, in $\text{Ni}_c\text{Fe}_{1-c}$. Open (C_d) and full squares (C_1) refer to the domain wall resistivities, open (C_0) and full (C_1) circles to "bulk" resistivities. Open and full up-triangles denote "bulk" resistivities when extending the fcc regime into the concentration range of the phase transition, open and full down-triangles those with respect to the bcc structure.

$$\rho_{CPP}(L; C_i, c) = \frac{1}{L} \iint_{-\infty}^{\infty} \rho(z, z'; C_i, c) dz dz' , \quad (5)$$

and the corresponding sheet resistance by

$$r(L; C_i, c) = L \rho_{CPP}(L; C_i, c) . \quad (6)$$

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

$$\rho_{CPP}(L; C_i, c) \sim \rho_{zz}(L; C_i, c) = \sigma_{zz}^{-1}(L; C_i, c) , \quad (7)$$

One can make use also of the fact that $r(L; C_i, c)$ is linear in L ,

$$r(L; C_i, c) = L \rho_{zz}(L; C_i, c) = a(C_i, c) + b(C_i, c)L . \quad (8)$$

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

$$0 < c < 1 : \lim_{L \rightarrow \infty} \rho_{zz}(L; C_d, c) = b(C_d, c) = \rho_{zz}(C_0, c) , \quad (9)$$

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

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. Eq. (10) 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.[13]

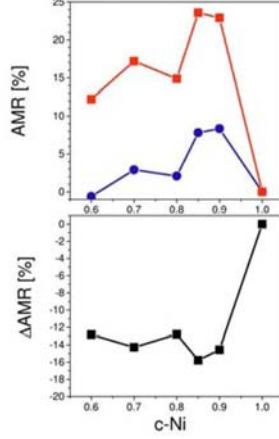


Figure 2: Top: "Bulk" (squares, Eq. (11)) and domain wall (circles, Eq. (12)) AMR in $\text{Ni}_c\text{Fe}_{1-c}$ for $0.6 \leq c \leq 1$. Bottom: Reduction of the AMR in the presence of a domain wall, see Eq. (13).

Clearly enough the "standard" expression for the anisotropic magnetoresistance [14] for bulk cubic systems, $0 < c < 1$, no longer makes sense in the presence of domain walls. However, one can define a similar ratio [15],

$$AMR(L_0; C_i, c) = \frac{\rho_{zz}(L_0; C_1, c) - \rho_{zz}(L_0; C_i, c)}{\rho_{zz}(L_0; C_1, c)}, \quad (11)$$

$C_i = C_0, C_d$, where L_0 now refers to the equilibrium domain wall width. Similarly, in the absence of domain walls use can be made of Eq. (9), i.e.,

$$AMR(c) = (\rho_{zz}(C_1, c) - \rho_{zz}(L_0; C_0, c)) / \rho_{zz}(C_1, c). \quad (12)$$

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

$$\Delta_{AMR} = AMR(L_0; C_i, c) - AMR(c), \quad (13)$$

which indicates how much the AMR is changed due to the presence of a domain wall. The definitions in Eqs. (11) and (13), however, only make sense - as already stated - if L_0 is sufficiently large.

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 $\text{Ni}_c\text{Fe}_{1-c}$ the effective potentials and exchange fields were calculated selfconsistently 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 $E(L; C_d, c)$ were evaluated by means of a contour integration along a semi-circle 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 [13] using also 1830 k points per ISBZ and then analytically continued to the real axis. It turns out that in using Eqs. (7) - (10) the inherent numerical errors are rather very small.

In the left part of Fig. 1 the experimental lattice constants and the calculated spin-only moments in $\text{Ni}_c\text{Fe}_{1-c}$ are displayed versus the Ni concentration. Note the very sharp break in the size of the lattice constants at

about 35% Ni, a break which also can be read off in the magnetic moments for Ni and Fe (lower panel). The concentration regime of the phase transition is usually listed in the literature to occur in about $0.25 \leq c \leq 0.45$.

In the upper right part of Fig. 1 the equilibrium domain wall width in $\text{Ni}_c\text{Fe}_{1-c}$ from Ref. [11] is shown, while in the lower part of this figure the resistivities $\rho(C_0, c)$ and $\rho(C_1, c)$, namely the so-called bulk residual resistivities, see Eq. (9), and the respective domain wall resistivities $\rho(L_0; C_1, c)$ and $\rho(L_0; C_d, c)$ are displayed versus the Ni concentration. As can be seen with decreasing L_0 the domain wall resistivities grow, leaving therefore only a narrow concentrational window for the "race tracking", namely a concentration regime with reasonably large $\Delta AMR(c)$, see Eqs. (11) - (13), which in turn is shown explicitly in Fig. 2.

Summary: It was shown by means of fully relativistic ab-initio calculations that in permalloy, $\text{Ni}_c\text{Fe}_{1-c}$, there is only a small concentration range in which in comparison to the corresponding "bulk" value the AMR (meaningfully defined) is reduced in the presence of a domain wall. This reduction is quite large, namely about 16% in the vicinity of 80% Ni.

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