Electric properties of generalized domain walls and spin spirals in permalloy

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In using the fully relativistic versions of the screened Korringa-Kohn-Rostoker method and of the Kubo-Greenwood equation for permalloy, $Ni_{85}Fe_{15}$, the equilibrium width of generalized domain walls and the corresponding resistivities are calculated for the case that the orientations of the magnetization in the two domains separated by a wall form a relative angle, which is assumed to vary continuously between 0° and 360°. It is found, e.g., that the width of a 90° domain wall is shorter by 100 nm than the one for a 180° domain wall yielding a reduction in the anisotropic magnetoresistance ratio (AMR), which as compared to the bulk value (no domain wall present) is even larger than that for a 180° domain wall. In particular it is demonstrated that the reduction in the AMR of generalized domain walls can safely be correlated with the anisotropy contribution to their formation energies.

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Recently, domain walls, in particular their current induced motions in permalloy have attracted a lot of attention. In an impressive series of papers, some of them only a few months old, Parkin *et al.*[1–6] demonstrated in terms of sophisticated experiments in what manner the old idea of storing information in movable domain walls can be put into a concept that eventually might lead to a completely new type of memories, namely to an all-solid-state device with no moving parts at all. Most recently[2] even the viability of a shift-register memory was shown and the possibility of three-dimensional "race track memories" discussed.[1] Clearly, if successfully applicable and technologically transferable an approach based on the current induced motion of domain walls would completely change the landscape of computer memories.

Up to now, however, it seems that the critical ("spin-polarized") current necessary to drive domain walls is still too large. Therefore, the idea was raised whether by changing the composition of Ni_xFe_{1-x},[7,8] or, by considering even a completely different system of alloys based on magnetic 3*d* elements[9] would result in a more attractive effect, namely an enhanced reduction in the anisotropic magnetoresistance ratio (AMR) in the presence of a domain wall. Unfortunately from fully relativistic *ab initio* studies[7–9] it turned out that the presently used alloy system namely permalloy with about 85% Ni is the best possible choice. Co_xNi_{1-x} and Fe_xCo_{1-x}, e.g., yielded a much inferior reduction in the AMR. In principle therefore—at least from a theoretical point of view—the only remaining possibility to improve the present materials specific setup is to modify the orientation in one magnetic domain relatively to the other one. This is exactly the problem addressed in the present Brief Report. For this matter (100) $Ni_{85}Fe_{15}$ is viewed as a two-dimensional translational invariant system (presently the best possible model to simulate nanowires on an *ab initio* level) with the direction of the magnetization in one magnetic domain and of the current being parallel to the surface normal (the setup used in the experiments by Parkin *et al.*[1–6]). In the other domain, however, the orientation of the magnetization varies continuously in a plane containing the surface normal causing thus "generalized" domain walls to be built up. By varying the relative angle Θ between the orientations of the magnetization in the two domains (described theoretically as semi-infinite systems) between 0° and 360° not only 90° and 180° domain walls can be studied but also "spin spirals."

Suppose that C_x refers to the following magnetic configuration,

$$C_x = \{\vec{n}_l = \vec{x},\ \ \vec{n}_i = \vec{x},\ \ \vec{n}_r = \vec{x},\ \ i = 1,\ \ L\}, \tag{1}$$

where $\vec{n}_l$ and $\vec{n}_r$ denote the orientations of the magnetization in the "left" and the "right" semi-infinite system, the $\vec{n}_i$ those in the L atomic planes of the remainder (domain wall), $\vec{x}$ ($\vec{y}$) is parallel to the in-plane x (y) axis, and $\vec{z}$ is parallel to the surface normal. Suppose further a magnetic configuration $C(\Theta)$ such that in the atomic layers in between the two semi-infinite systems the orientation of the magnetization in the individual planes changes continuously from $\vec{z}$ to $D(\Theta)\vec{z}$,

$$C(\Theta) = \{\vec{n}_l = \vec{z},\ \ \vec{n}_i,\ \ \vec{n}_r = D(\Theta)\vec{z},\ \ i = 1,\ \ L\}, \tag{2}$$

$\vec{n}_i = D(\vartheta_i)\vec{z}$, $\vartheta_i = (i/L)\Theta$, $i = 1, \ldots, L$, $D(\vartheta_i)$ being a rotation by an angle ϑ_i around the y axis. Equation (2) denotes a noncollinear magnetic structure in which the orientations of the magnetization in all atomic planes lie in the (x,z) plane, those in the left and the right semi-infinite system forming a (uniform) relative angle Θ. Clearly, configuration $C(90)$ corresponds to a 90° domain wall and $C(360)$ to a "spin spiral" of length L (in monolayers), or, viewed differently, corresponds to a "head" to "tail" arrangement of two subsequent 180° domain walls.

For a particular value of L the formation energy $E(L;\Theta)$ can be evaluated via the magnetic force theorem as the difference in the grand canonical potentials of $C(\Theta \neq 0)$ and $C(\Theta = 0)$.[7,10] In using a multiscale approach this formation energy can be written as

$$E(L;\Theta) = A_0[\alpha(\Theta)/L + \beta(\Theta)L], \tag{3}$$

where A_0 refers to the unit area, and the constants $\alpha(\Theta)$ and $\beta(\Theta)$ correspond in turn to the exchange and anisotropy energy. Clearly in assuming this form the parameters, $\alpha(\Theta)$ and $\beta(\Theta)$ have to be independent of pairs of points chosen at which $E(L;\Theta)$, $0 \leq \Theta \leq 360°$ is evaluated.[9] The position of the minimum of $E(L;\Theta)$, $L_0(\Theta) = \sqrt{\alpha(\Theta)/\beta(\Theta)}$ is then usu-

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ally referred to as the equilibrium width of a domain wall or equilibrium length of a spin spiral.

Applying a current perpendicular to the planes of atoms (CPP) the resistivity $\rho_{\mathrm{CPP}}(L;C)$ defined over a large enough L [9,11] and for a particular magnetic configuration C can be obtained from the zz component of the conductivity tensor, whereby use can made of the fact that the sheet resistance $r(L;C)=L\rho_{zz}(L;C)$ is linear in L,[12]

$$r(L;C) = a(C) + b(C)L. \qquad (4)$$

At the equilibrium width (length) $L_0(\Theta)$ the following anisotropic magnetoresistance ratio (AMR) can now be defined:

$$\mathrm{AMR}(L_0;\Theta) = \Delta\rho_{zz}(L_0;\Theta)/\rho_{zz}[L_0;C(\Theta)], \qquad (5)$$

$$\Delta\rho_{zz}(L_0;\Theta) = \rho_{zz}[L_0(\Theta);C(\Theta)] - \rho_{zz}[L_0(\Theta);C_x]. \qquad (6)$$

For $\Theta=0$ this definition refers to the case that no noncollinear structure (domain wall or spin spiral) is present in between the two electric contacts separated by $L_0(\Theta)$, needed to record resistances, i.e., at $\Theta=0$ a bulklike AMR is present. It should be noted that like in Eq. (6) in the following also an abbreviated notation for the equilibrium domain-wall formation energies will be used, namely $E(L_0;\Theta)$ instead of $E[L_0(\Theta);C(\Theta)]$.

All *ab initio* calculations for $Ni_{85}Fe_{15}$ were performed at the experimental lattice constant ($a_0=6.695$ a.u.) in terms of the spin-polarized relativistic screened Korringa-Kohn-Rostoker (SPR-KKR) method within the framework of the inhomogeneous coherent potential approximation.[13] In using the self-consistent potentials and exchange fields corresponding to configuration $C(0)$ the grand potentials $E(L;\Theta)$ were evaluated by means of a contour integration along a semicircle using a 16-point Gaussian quadrature and 1830 k points per irreducible part of the surface Brillouin zone (ISBZ). It turned out that by choosing in Eq. (3) different pairs of points with increasing averaged length the corresponding equilibrium lengths $L_0(\Theta)$ differed by less than 2% for all relative angles Θ considered. The electric transport properties were evaluated at complex Fermi energies by means of the fully relativistic Kubo equation[12] using also 1830 k points per ISBZ and then analytically continued to the real axis.

Figure 1 shows the formation energy $E(L;\Theta)$ for four different lengths L with Θ varying between 0° and 360°. As can be seen with increasing L the slope of $E(L;\Theta)$ with respect to Θ becomes flatter and—as to be expected—corresponding formation energies are reduced in value. In displaying $E(L;\Theta)$ as a function of L at given values of Θ, see Fig. 2, at the first glance a surprising feature of the minima in $E(L;\Theta)$ appears: the $E(L_0;\Theta)$ are points of a line which eventually has to pass through zero, since $E(L;0)=0, \forall L$. The second feature is perhaps less surprising, namely that with increasing relative angle Θ between the two semi-infinite systems the minima in the $E(L;\Theta)$ versus L curves become increasingly flatter.

In Fig. 3 the parameters $\alpha(\Theta)$ and $\beta(\Theta)$, namely the exchange and the anisotropy energy, are shown versus Θ together with the equilibrium length $L_0(\Theta)$. As can be seen

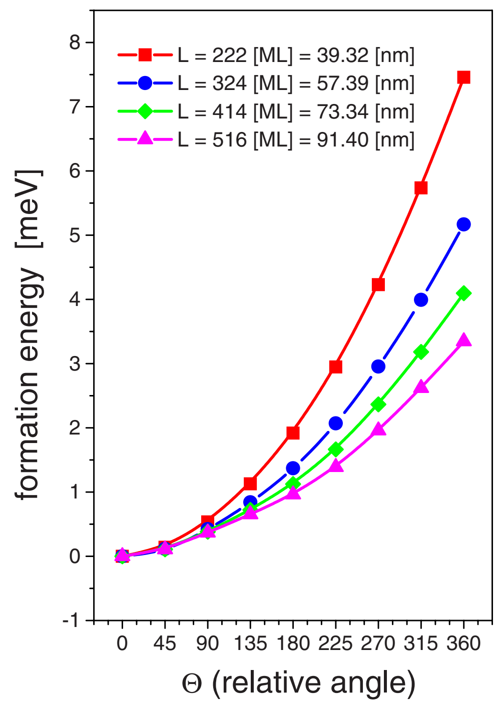

FIG. 1. (Color online) Formation energy of the noncollinear structures at various lengths (widths, indicated in the figure) as a function of the relative angle Θ between the two magnetic domains.

while the exchange energy changes (nearly) parabolically with increasing Θ, the anisotropy parameter has two maxima, namely at 135° and 315°, separated by a minimum at 225°, the values at 90°, 180°, 270° and 360° being almost the same. The consequences of the changes in $\alpha(\Theta)$ and $\beta(\Theta)$ with respect to Θ for the equilibrium length $L_0(\Theta)$ can

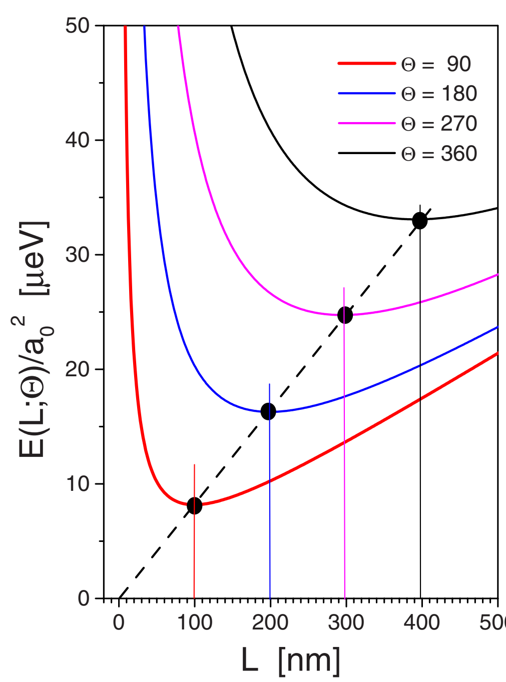

FIG. 2. (Color online) Formation energy $E(L;\Theta)$ versus the width L for selected values of Θ.

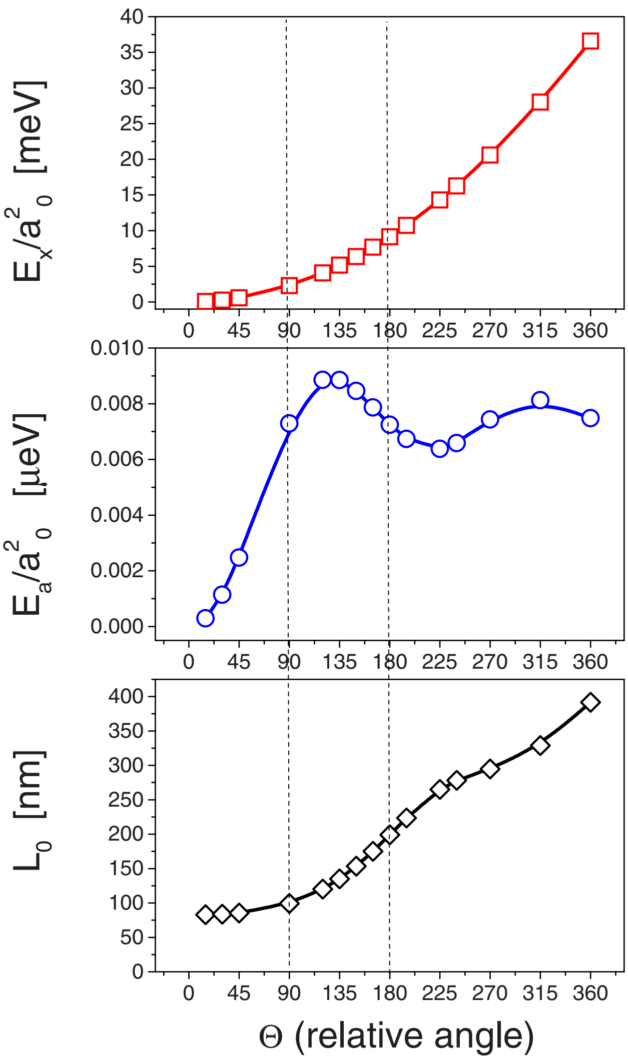

FIG. 3. (Color online) Exchange energy (top), anisotropy energy (middle), and equilibrium width versus the relative angle Θ between the two semi-infinite systems. The area between the two dashed, vertical lines highlights the regime of angles between 90° and 180° domains.

be read off from the bottom part of Fig. 3. There seem to be two regimes of rapid changes in $L_0(\Theta)$, namely one corresponding to about $90° \leq \Theta \leq 225°$ and the other one referring to $270° \leq \Theta \leq 360°$, the technologically interesting being of course the first one. The equilibrium width of a 90° domain wall is about half of that of a 180° domain wall. Expressed in absolute numbers this difference amounts to about 100 nm. This reduction in length indicates that a 180° domain wall can be viewed as a "head" to "tail" arrangement of two 90° domain walls.

Turning now to the second type of results, namely to $\Delta\rho_{zz}(L_0;\Theta)$ and $\text{AMR}(L_0;\Theta)$, defined in Eqs. (5) and (6), one can see from Fig. 4 that the changes with respect to Θ are quite dramatic. At $\Theta=90°$ there is a minimum in $\Delta\rho_{zz}(L_0;\Theta)$, while for values of $\Theta \geq 180°$ this difference is about constant. The minimum in $\Delta\rho_{zz}(L_0;\Theta)$ causes of course a dramatic drop in the magnetoresistance ratio. While for $\Theta=0$ (no domain wall or spin spiral present) the AMR amounts to about 18%, for a 180° domain wall (and for

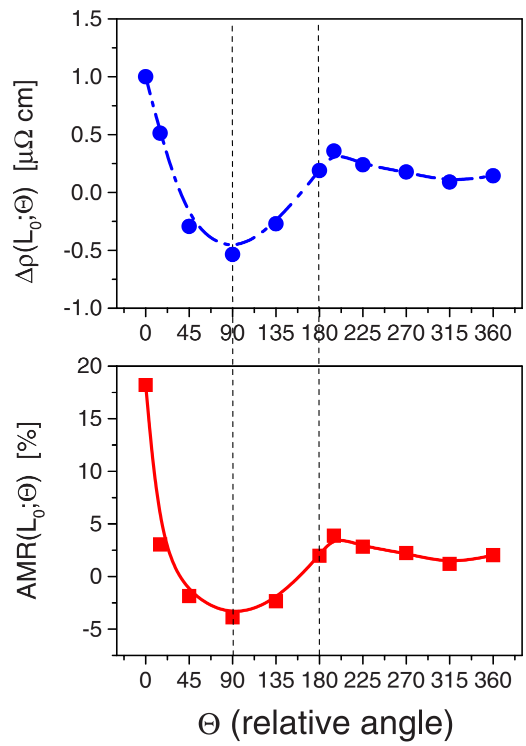

FIG. 4. (Color online) Difference in resistivities, see Eq. (6) and corresponding anisotropic magnetoresistance as defined in Eq. (5) versus the relative angle Θ between the two semi-infinite systems.

higher twisted noncollinear structures, $\Theta \geq 180°$) it drops to about 2%; i.e., the presence of such a domain wall or spin spiral causes a reduction in the AMR of about 16%. For $\Theta=90°$, however, the usual AMR effect in permalloy is not only completely whipped out, but also slightly reversed; the reduction amounts to 22%. It is obvious from Fig. 4 that there are two different regimes: one for $\Theta \leq 180°$, the other one for $\Theta > 180°$, in which the reduction in the AMR remains about constant although the equilibrium length $L_0(\Theta)$ increases steadily.

The last bit of information needed to judge whether twisting the orientation of the magnetization in one of the domains can be used as an improvement of present setups for current induced domain-wall motions is the variation of the actual resistivities with respect to the equilibrium length $L_0(\Theta)$. From Fig. 5 one easily can see that with decreasing equilibrium length all of the depicted resistivities increase rapidly. The reason for this perhaps unwanted behavior is easily understood from Eq. (4), namely from the definition of the resistivities via sheet resistances. Since for $\Theta=0$ only one uniform orientation of the magnetization applies to the whole infinite system consisting "artificially" of two semi-infinite parts in Fig. 5 for comparison the corresponding "bulk" values are displayed, which were also used for the entry at $\Theta=0$ in Fig. 4.

Turning now explicitly to the regime of spin spirals, i.e., to $\Theta > 180°$, two interesting features can be pointed out, namely (1) a "classical" spin spiral ($\Theta=360°$) in permalloy seems to be only very shallowly bound with an equilibrium length of about 400 nm, and (2) a comparison between Figs. 3 and 4 indicates that also in this regime the shape of the

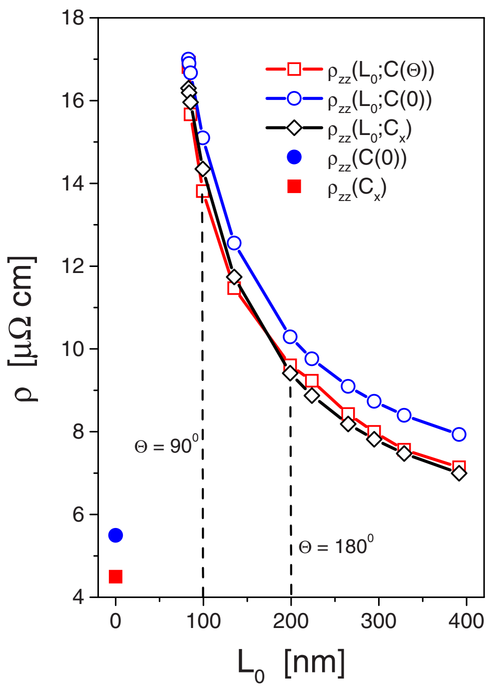

FIG. 5. (Color online) Resistivities $\rho_{zz}[L_0;C(\Theta)]$, $\rho_{zz}[L_0C(0)]$, and $\rho_{zz}(L_0;C_x)$ versus the equilibrium width L_0. For comparison also the "bulk" values of $\rho_{zz}[C(0)]$ and $\rho_{zz}(C_x)$ are shown. The vertical dashed lines indicate the values at $\Theta=90°$ and 180°, respectively.

curve reflects (inversely) that for the anisotropy energy: at a maximum of the anisotropy energy the AMR has a minimum. The driving force for a reduction in the AMR in the presence of a domain wall or spin spiral when compared to the bulk case seems to be correlated with the anisotropy contribution to the equilibrium formation energy of the particular noncollinear structure placed between two domains whose orientations of the magnetization are noncollinearly aligned.

It is important to note that by construction, see Eq. (2), $E(L,\Theta)\neq E(L,360-\Theta)$ and therefore also the corresponding resistivities are different. This inequality has nothing in common with a chirality effect which would distinguish between a clockwise and a counterclockwise rotation by one and the same angle. Such an effect might be accessible when lifting inherent time inversion symmetries by means of an appropriate external field.

In summary it was shown that by monitoring the relative angle between two adjacent domains not only the equilibrium width of the domain wall separating these two domains can be reduced considerably, but also the reduction in the AMR is substantially enhanced, however, at the expense that relevant resistivities increase in value. Whether or not this finding can be used fruitfully for an improvement of "race track memories" will have to turn out. Furthermore, by considering also electric transport properties of spin spirals it was demonstrated that the main driving force for the reduction in the AMR most likely can be correlated with the anisotropy term in the formation energy of generalized magnetic domain walls.

Not considered in here was the actual interaction of an external electromagnetic field with a magnetic system (necessary to drive a domain wall) by using the time-dependent Dirac equation,[14] a concept, which, although offering in principle the possibility to evaluate all occurring torque terms rigorously, might take quite some time to be put into a practicable computational scheme based on an *ab initio* level.[15]

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