

Magnetostatic coupling in spin valves: Revisiting Néel's formula

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We use a numerical, atomistic approach to calculate the magnetostatic coupling in spin valves. In addition to the numerical treatment, the coupling energy is evaluated analytically and it is shown that Néel's formula is accurate to first order in the ratio of roughness amplitude to grain size. We also generalize the formula so that it can be applied to systems such as Py/Co/Cu/Co/Py spin valves that have complex ferromagnetic layers. © 2000 American Institute of Physics.
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I. INTRODUCTION

The two ferromagnetic (FM) layers in spin valve type trilayers (magnetic heterostructures consisting of two ferromagnetic films separated by a nonmagnetic spacer) tend to couple ferromagnetically. In many cases this coupling is attributed to the roughness of the interfaces on both sides of the nonmagnetic spacer and the magnetic charges that form as a consequence of this roughness.¹⁻³ Since this roughness is often correlated, especially when film growth is by columnar grain growth of the spin valve stack (Fig. 1), the magnetostatic interactions between the charges favor parallel alignment of the respective magnetizations of the two FM layers. This coupling is known as orange peel coupling (OPC) or Néel coupling. In the early 1960s Néel,⁴ following a suggestion by Metfessel,⁵ calculated the magnetostatic energy of two semi-infinite ferromagnetic layers A and A' that separated by a vacuum region B such that the interfaces $A-B$ and $B-A'$ are assumed to have a two dimensional waviness of the form

$$z(x,y) = -h \sin \frac{2\pi x}{\lambda} \sin \frac{2\pi y}{\lambda}. \quad (1)$$

In his calculation, Néel projected the magnetic charge distribution that results from the waviness onto the xy plane and solved for the magnetostatic energy (per unit area) of two FM layers with charged interface planes. For the case in which the magnetization in both FM layers is rigid,⁶ the solution for parallel alignment of the FM layers is

$$E_{\uparrow\uparrow} = \frac{\pi^2}{\sqrt{2}} M_s M'_s h h' e^{-2\pi d \sqrt{2}/\lambda}, \quad (2)$$

where M_s and M'_s represent the saturation magnetizations of the FM layers A and A' , respectively. The magnetostatic energy for antiparallel alignment of the FM layers is $E_{\uparrow\downarrow} = -E_{\uparrow\uparrow}$.

The assumption that the FM magnetization is rigid is justified since the grain sizes in typical spin valves are not much larger than the exchange length of the FM materials involved. However, it is not clear how valid the assumption is of a flat distribution of charges for the case in which the amplitude of the roughness h is of the same order of magni-

tude as the thickness d of the nonmagnetic spacer (typical values in spin valve applications $h=0.5-1$ nm and $d=2$ nm).

In the present work we take an atomistic approach to calculate the OPC which does not make any assumption about the topology of the interfacial charge distribution. We derive expressions for the magnetostatic energy that can be evaluated numerically and we use an approximate analytic evaluation of these expressions to derive Néel's formula. The direct comparison of numerical and analytical results gives a clear understanding of the range of validity of Néel's formula and indicates how OPC can be included in micromagnetic models of spin valves. This last point is particularly important because present micromagnetics models neglect interfacial roughness even though the OPC related coupling field can be as large as 10 Oe,^{1,2} which is comparable to other characteristic fields that appear in spin valves.⁷

II. NUMERICAL APPROACH

For the numerical treatment we assume that the FM is composed of localized atomic moments \mathbf{m}_i that are situated on atomic sites i with position vectors \mathbf{R}_i . Furthermore we choose models for the interface roughness in such a way that the film is two dimensional (2D) periodic in the xy plane. The magnetization can thus be written as

$$\mathbf{M}(\mathbf{r}) = \sum_i \frac{\mathbf{m}_i}{V_i} \sum_{\mathbf{R}} \delta[\mathbf{r} - (\mathbf{R}_i + \mathbf{R})], \quad (3)$$

where \mathbf{R} are the 2D lattice vectors, V_i represents the volume of the i th atomic cell, and the i summation runs over all sites in the unit cell. The magnetostatic energy per unit area is then given by

$$E = -\frac{1}{2\Omega} \sum_{i \neq j} \mathbf{m}_i \mathbf{D}_{ij} \mathbf{m}_j, \quad (4)$$

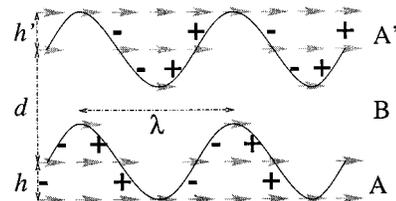


FIG. 1. Schematic of two FM layers with correlated wavy surfaces. Arrows indicate positions of atomic moments.

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where Ω is the area of the unit cell, and the dipolar interaction matrix is given by

$$(\mathbf{D}_{ij})_{\mu\nu} = \sum_{\mathbf{R}} \frac{3(\hat{\mathbf{n}}_i)_\mu(\hat{\mathbf{n}}_j)_\nu - \delta_{\mu\nu}}{|\mathbf{R}_i - \mathbf{R}_j - \mathbf{R}|^3} \quad (5)$$

with $\hat{\mathbf{n}}_i = \mathbf{R}_i/|\mathbf{R}_i|$ and $\mu(\nu)$ labeling Cartesian coordinates.

The OPC is usually extracted from a positive offset, H_o in the magnetization loop of the free layer f of the spin valve.¹ In our atomistic approach, when all moments in a layer are parallel,

$$H_o = \frac{J}{\left(\sum_{i \in f} \frac{m_i}{V_i}\right) t_f}, \quad (6)$$

where t_f is the thickness of the free layer and

$$J = (E_{\downarrow\downarrow} - E_{\uparrow\uparrow}) \quad (7)$$

is the coupling energy between the layers. Since the sum in Eq. (5) is conditionally convergent a few more transformations are required before Eqs. (4), (5), and (7) can be evaluated numerically.

In the present work we assume that $d > 2h$ so that $|\mathbf{R}_i - \mathbf{R}_j| \neq 0$, when the sites i and j are not in the same FM layer. Since, in the case for which the magnetization of an individual layer FM is rigid, the only contributions to the magnetostatic energy [Eq. (4)] that do not cancel in Eq. (7) are those for which i and j are in different layers, we can calculate the sums in Eq. (5) with Fourier transforms. Assuming that the magnetization points along the x axis we get

$$J = \frac{1}{\Omega} \sum_{i \in A, j \in A'} m_i (D_{ij})_{xx} m_j, \quad (8)$$

where

$$(D_{ij})_{xx} = -\frac{2\pi}{\Omega} \sum_{\mathbf{G} \neq 0} e^{-G|R_{i,z} - R_{j,z}|} \frac{G_x^2}{G} \cos[\mathbf{G}(\mathbf{R}_i - \mathbf{R}_j)]. \quad (9)$$

Evidently, this last expression converges whenever $|R_{i,z} - R_{j,z}| > 0$. For the case of a distribution of moments on a square lattice, the reader can verify that this expression reduces to the result obtained by Tsymbal.⁸

III. APPROXIMATE ANALYTIC TREATMENT

To derive Néel's OPC result from the expressions given in Sec. II, we begin by calculating the field at some site \mathbf{r} (with $r_z > h$) due to magnetic moments which are situated below the surface

$$z(x, y) = h \left(\sin^2 \frac{\pi x}{L} \cos^2 \frac{\pi y}{L} - \cos^2 \frac{\pi x}{L} \sin^2 \frac{\pi y}{L} \right). \quad (10)$$

Note that Eqs. (1) and (10) are equivalent when $\lambda = \sqrt{2}L$. In accordance with the assumptions that lead to Eq. (2), we can assume here that all the moments vectors are identical and point along the x axis, i.e., $\mathbf{m}_i = m\hat{\mathbf{x}}$ and $M_s = m/V$. Using Eq. (9) we have for the x component of the magnetostatic field

$$H_x = -\frac{2\pi}{\Omega} M_s \sum_{\mathbf{G} \neq 0} \frac{G_x^2}{G} \sum_i e^{-G|r_z - R_{i,z}|} \cos[\mathbf{G}(\mathbf{r} - \mathbf{R}_i)]. \quad (11)$$

The first approximation we make is to retain only the first shell in the reciprocal lattice sum and replace the summation over sites by integrals. This converts Eq. (11) to

$$H_x = -\frac{8\pi^2 e^{-r_z 2\pi/L}}{\Omega L} M_s \int_0^L dx dy \cos\left(\frac{2\pi}{L}(r_x - x)\right) \times \int_{-h}^{z(x,y)} dz' e^{z' 2\pi/L}. \quad (12)$$

The z integral yields an exponential function which we evaluate only to first order in (h/L) , i.e.,

$$\int_{-h}^{z(x,y)} dz' e^{z' 2\pi/L} = \frac{L}{2\pi} (e^{z(x,y) 2\pi/L} - e^{-h 2\pi/L}) = [z(x,y) + h] + o(h/L)^2. \quad (13)$$

Note that this is the second approximation which we made. The remaining integrals in Eq. (12) are now straightforward to evaluate and we find

$$H_x = 2\pi^2 M_s \frac{h}{L} \cos \frac{2\pi R_x}{L} e^{-R_z 2\pi/L}. \quad (14)$$

An analogous expression can be obtained for the field at a site with $R_z < d - h$ due to moments situated on sites above $z(x, y) + d$.

Using this last result to calculate the magnetostatic self energy $E = -1/(2\Omega) \int M H d^3 r$ (where we again replace the summation over moment by an integral) for the parallel and antiparallel states of the spin valve, we get, after exploiting all possible symmetries,

$$J = \frac{4\pi^2}{\Omega} M_s^2 \frac{h}{L} \int_0^L dx dy \cos \frac{2\pi x}{L} \int_{d+z(x,y)}^\infty dz e^{-z 2\pi/L} + o(h/L)^2. \quad (15)$$

Repeating the steps which lead from Eq. (12) to Eq. (14) yields the final result for the coupling energy

$$J = \sqrt{2} \pi^2 M_s^2 \frac{h^2}{\lambda} e^{-2\pi\sqrt{2}d/\lambda} + o(h/\lambda)^2, \quad (16)$$

where we have replaced L by $\lambda = L/\sqrt{2}$. This formula is equivalent to the combination of Néel's formula, Eq. (2), and Eq. (4).⁹

IV. DISCUSSION

The results of Eqs. (8) and (16) are compared in Fig. 2. For the numerical treatment we have assumed two 8 nm thick Permalloy films for which, for simplicity, we assume that atomic moments of $1\mu_B$ occupy a simple cubic lattice with lattice constant $a = 2.25 \text{ \AA}$ and that interface planes are parallel to (001). The interfaces with the spacer layer have a sinusoidal waviness of the form discussed in Sec. II and the outer surfaces are flat. This is a very accurate model of two semi-infinite FM slabs, because the contributions of perfect

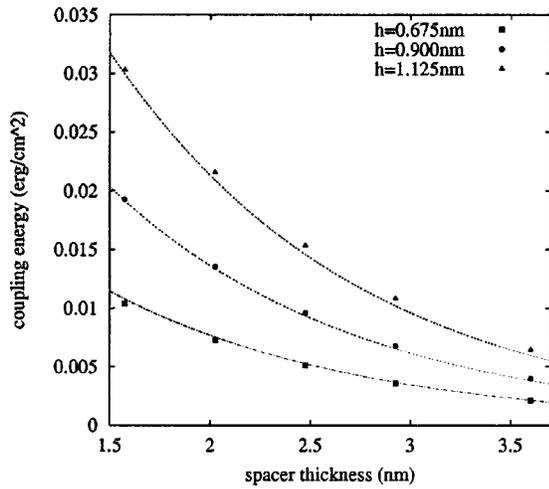


FIG. 2. Numerical evaluation of coupling energy (symbols) compared with results of Eq. (16) as a function of spacer thickness for different roughness amplitudes. Results are for $L = \lambda/\sqrt{2} = 7.875$ nm.

layers to the energy fall off with a factor $-2\pi|z|/a$ instead of $-2\pi|z|/L$ in the exponential of Eq. (9). The results in Fig. 2 confirm our expectations from the derivation of Néel's formula in Sec. III: Independent of the spacer thickness, the agreement is best for the smallest values of h but the deviations are still small for values $h \approx 1$ nm since the error is of order $(h/L)^2$.

The formulas of Sec. II are valid for any distribution of magnetic moments in the unit cell and are thus applicable to inhomogeneous films. It is also straightforward to generalize the analytic derivation of Sec. III to the case of multiple FM layers. For the important case of spin-valve applications, where Co is introduced as a diffusion barrier between Py and the Cu on both sides of the spacer, one has to consider a Py/Co/Cu/Co/Py multilayer. For this case the coupling energy is (to first order in h/L)

$$J = \frac{\pi^2}{L} h^2 e^{-(2\pi d/L)} (M_{Py})^2 \left\{ \left(\frac{M_{Co}}{M_{Py}} \right)^2 [1 - e^{-(2\pi/L)t_2} - e^{-(2\pi/L)t_3} + e^{-(2\pi/L)(t_2+t_3)}] + \frac{M_{Co}}{M_{Py}} e^{-(2\pi/L)t_2} \times [1 - e^{-(2\pi/L)t_1} - e^{-(2\pi/L)t_3} + e^{-(2\pi/L)(t_1+t_3)}] + \frac{M_{Co}}{M_{Py}} e^{-(2\pi/L)t_3} [1 - e^{-(2\pi/L)t_2} - e^{-(2\pi/L)t_4} + e^{-(2\pi/L)(t_2+t_4)}] + e^{-(2\pi/L)(t_2+t_3)} [1 - e^{-(2\pi/L)t_1} - e^{-(2\pi/L)t_4} + e^{-(2\pi/L)(t_1+t_4)}] \right\},$$

where t_i represent the respective thicknesses of the FM layers in the stack Py/Co/Cu/Co/Py. For simplicity we have assumed that all interfaces have the same roughness amplitude. Results for the corresponding offset field are illustrated in Fig. 3, from which one concludes that, in order to reduce the OPC related offset, the Co diffusion barrier should be kept as thin as possible. This is because the magnetic charges at the Co/Py interfaces are anticorrelated with the charges at

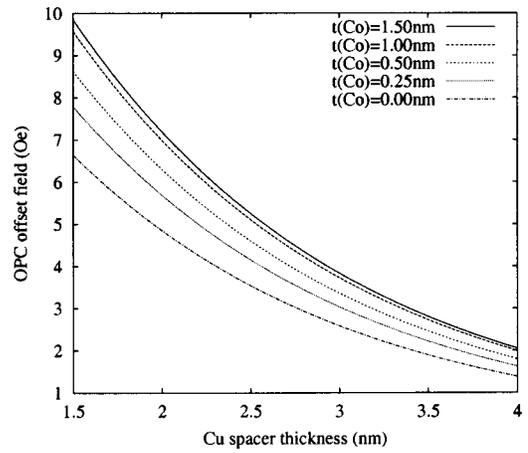


FIG. 3. OPC offset field for a Py(3 nm)Co(t_{Co})/Cu/Co(t_{Co})/Py(3 nm) spin valve with a double sinusoidal waviness of amplitude $h = 0.3$ nm on all interfaces. Results are for $L = \lambda/\sqrt{2} = 10$ nm.

the Co/Cu interface on the other side of the spacer and thus cancel the OPC. A similar result was found for the case of very thin homogeneous FM layers by Zhang and White¹⁰ numerically and by Kools *et al.*¹¹ in terms of Néel's model.

In summary, we have investigated the magnetostatic coupling due to correlated roughness in spin valves both numerically and analytically. The derivation and the numeric examples show that Néel's formula is correct to first order in h/λ . A generalization for Py/Co/Cu/Co/Py spin valves has been given, which shows that in order to reduce the OPC offset field, the Co diffusion barrier should be kept as thin as possible.

ACKNOWLEDGMENT

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