

Calculation of CPP- and CIP-magnitoresistance in multilayer magnetic structures

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Abstract. A Monte Carlo simulation of magnetic properties for structures Fe/Cr/Fe and Co/Cu/Co, constructed from two ferromagnetic films divided by nonmagnetic film are carried out. The calculation of the magnetoresistance is carried out in case of CPP and CIP geometry for different thicknesses of the ferromagnetic films with the use of the anisotropic Heisenberg model for determination of magnetic properties. It was shown, that the obtained temperature dependence for the magnetoresistance agrees very well with experimental results.

1 Introduction

The artificial created multilayer magnetic superlattices has become of great interest for wide range of applications based on the phenomena of the giant magnetoresistance (GMR) and the tunneling magnetoresistance. Devices based on the GMR effect are widely used as read heads of hard disks, memory devices, sensors, etc [1]. Achievements in the development of technology give possibility now to receive a high-quality ultrathin films and multilayer coatings on the basis of the magnetic transition metals Fe, Co, and Ni. The magnetic properties of ultrathin films and superstructures are sensitive to the effects of anisotropy generated by the crystal field of a substrate or nonmagnetic layers. Therefore, the physical properties of ultrathin films based on Fe, Co, and Ni can be described by the anisotropic Heisenberg model [2, 3].

We developed in [4, 5] a new methodology for determination of the magnetoresistance (MR) with the use of the Monte Carlo method for measurements of MR with the current perpendicular to plane (CPP – MR). The magnetoresistance had been calculated for three-layer and spin-valve magnetic structures at various thicknesses of ferromagnetic films. It had been shown that the calculated temperature dependence of the magnetoresistance is in good agreement with experimental data obtained for the Fe(001)/Cr(001) multilayer structure and the CFAS/Ag/CFAS/IrMn spin valve based on the $\text{Co}_2\text{FeAl}_{0.5}\text{Si}_{0.5}$ (CFAS) Heusler alloy.

In this paper, we expand our methodology [4] for determination of MR in case of measurements with the current in plane (CIP–MR). We introduce for calculation of the CIP-MR a phenomenological parameter of electron scattering at F/N interfaces. The parameter of scattering can be determined from comparison of calculated and experimentally measured CIP-MR values

for Fe/Cr(100)/Fe and Co/Cu(100)/Co multilayer structures [6].

2 Model and methods

We use the Hamiltonian of the anisotropic Heisenberg model [4, 5] for the Monte Carlo statistical description of the magnetic properties of Fe films for Fe/Cr(100)/Fe multilayer structure with the out of plane magnetization in Fe films

$$H = - \sum_{\langle i,j \rangle} J_{ij} \{ (1 - \Delta_1(N)) (S_i^x S_j^x + S_i^y S_j^y) + S_i^z S_j^z \}, \quad (1)$$

and for Co films in Co/Cu(100)/Co multilayer structure with the in plane magnetization in Co films

$$H = - \sum_{\langle i,j \rangle} J_{ij} \{ (S_i^x S_j^x + S_i^y S_j^y) + (1 - \Delta_2(N)) S_i^z S_j^z \}. \quad (2)$$

Therein, J_{ij} characterizes the short-range exchange interaction between the spins S_i , fixed at the sites of a body-centered cubic (bcc) lattice for Fe films and face-centered cubic (fcc) lattice for Co films. $S_i = (S_i^x, S_i^y, S_i^z)$ is introduced as a three-dimensional unit vector. $\Delta_{1,2}(N)$ are an anisotropy parameters. The dependence of the anisotropy parameters $\Delta_{1,2}(N)$ on the film thickness N was selected as proportional to the experimental critical temperatures for Fe/Cr(100) and Co/Cu(100) systems [7, 8], and the curves of $\Delta_{1,2}(N)$ are given in Figure 1.

We considered a multilayer structure, which consists of two ferromagnetic films separated by a nonmagnetic metal film (Figure 2). The simulations were performed for the films with linear sizes $L \times L \times N$ with applied of the periodic boundary conditions in the film plane. $\nu L \times L$ gives the number of spins in each layer, where ν is the number of atoms in unit cell, and N is the number of monolayers in the thin film. We considered Fe/Cr system as bcc-structure with $\nu = 2$ and Co/Cu as fcc-

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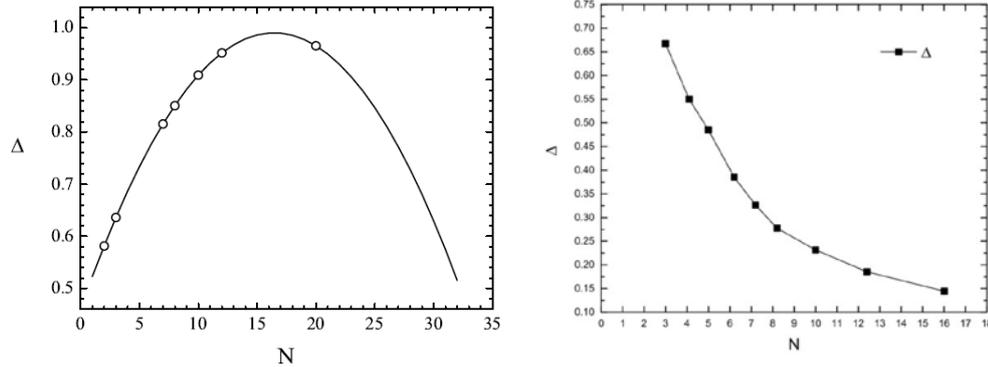


Fig. 1. The dependence of the anisotropy parameters $\Delta_1(N)$ (a) and $\Delta_2(N)$ (b) on thickness of the ferromagnetic film N in units of monatomic layers (ML). The circles are experimental data for Fe/Cr(100) (a) and Co/Cu(100) (b) systems.

structure with $\nu = 4$. The value of the exchange integral that determines the interaction of neighbouring spins inside the ferromagnetic film is specified as $J_1 > 0$ and the interaction between the films is taken as $J_2 = -0.1J_1$. The temperature T of the system is measured in units of the exchange integral J_1/k_B . Since $J_2 < 0$, the two films in the structure are magnetized in the opposite direction (one up and the other down). The spin configurations of the Heisenberg ferromagnetic films in the structures are updated using the Swendsen-Wang cluster algorithm.

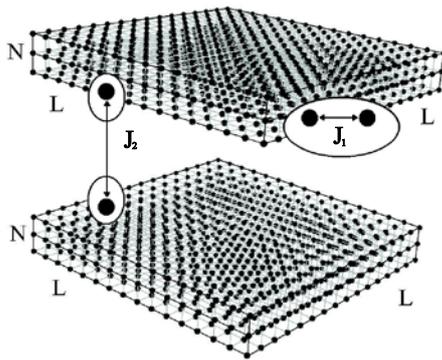


Fig. 2. Model of a multilayer structure consisting of two ferromagnetic films separated by the nonmagnetic metal film; L and N are the linear sizes of the films, J_1 and J_2 are the exchange integrals.

We calculated the magnetoresistance for a multilayer structures which is introduced as

$$\delta_h = \frac{R_{AP} - R_P}{R_P}, \quad (3)$$

where R_{AP} is the resistance of the structure when the magnetizations of adjacent ferromagnetic layers are aligned antiparallel, and R_P is the resistance of the structure for parallel orientation of the magnetization of ferromagnetic layers. The multilayer structure can connect two ways in the current line for measurements of the resistance: first case with the current in plane (CIP), when the current conduction is realized along layers and the electrodes are situated on one side of the structure, and second case with the current perpendicular to plane (CPP), when the current conduction is realized perpendicular to the layers of the superstructure and the electrodes are situated on both sides of the structure. It was shown in [6] that the CPP-MR is characterized by larger values than the CIP-MR, approximately twice as high, and becomes more competitive as the device size

shrinks. Now this method has great practical interest because the CPP-MR sensors demonstrate more sensitivity than CIP-MR sensors.

3 Methodology and results of calculation of CPP- and CIP-MR

We present in this section the methodology which was developed for the calculation of magnetoresistance in multilayered structures in case of CPP and CIP geometry. We denote the resistance of an ferromagnetic film for two groups of electrons with spins up R_\uparrow and spin down R_\downarrow . Here we use the simple two-current Mott model for the description of the resistance of different conductance channels. This model suggests conservation of orientation of electron spin moments during penetration of the structure and better corresponds to measurements of the CPP-MR. The total resistance of the trilayer structure (Fig. 2) for the antiparallel configuration, which is realized in the absence of a magnetic field, is determined by the relation $R_{AP} = (R_\uparrow + R_\downarrow)/2$. The parallel configuration of the trilayer structure for the magnetic field $H \geq H_s$, where H_s is saturation field, is characterized by the resistance in the form $R_P = (2 R_\uparrow R_\downarrow)/(R_\uparrow + R_\downarrow)$. Consequently, the magnetoresistance of the trilayer structure is determined by the relation

$$\delta_h = \frac{(R_\uparrow - R_\downarrow)^2}{4R_\uparrow R_\downarrow} = \frac{(J_\uparrow - J_\downarrow)^2}{4J_\uparrow J_\downarrow}, \quad (4)$$

where $\mathbf{J}_{\uparrow,\downarrow} = en_{\uparrow,\downarrow} \mathbf{V}_{\uparrow,\downarrow}$ is the current density. Here, $n_{\uparrow,\downarrow}$ is the density of electrons with z components of spin moment equal to $+1/2$ and $-1/2$, $n = n_\uparrow + n_\downarrow$ is the total electron density and $\mathbf{V}_{\uparrow,\downarrow}$ are the averaged velocities of electrons with corresponding spin projections. The electron densities with spin up and down can be expressed through the magnetization of the film $n_{\uparrow,\downarrow}/n = (1 \pm m)/2$ determined in the process of the Monte Carlo simulation. The averaged electron velocity $\mathbf{V}_{\uparrow,\downarrow}$ can be expressed through the electron mobility and the external electric field intensity \mathbf{E} , and after that through the probability of electron displacement in unit time (corresponding to one Monte Carlo step per spin) from unit cell i to a neighbouring unit cell in the direction of the electric field with averaging over all film unit cells:

$$\langle V_{\uparrow,\downarrow} \rangle = \mu_{\uparrow,\downarrow} E = \frac{e}{T} E e^{-\frac{\Delta E_{i,\uparrow,\downarrow}}{T}}, \quad (5)$$

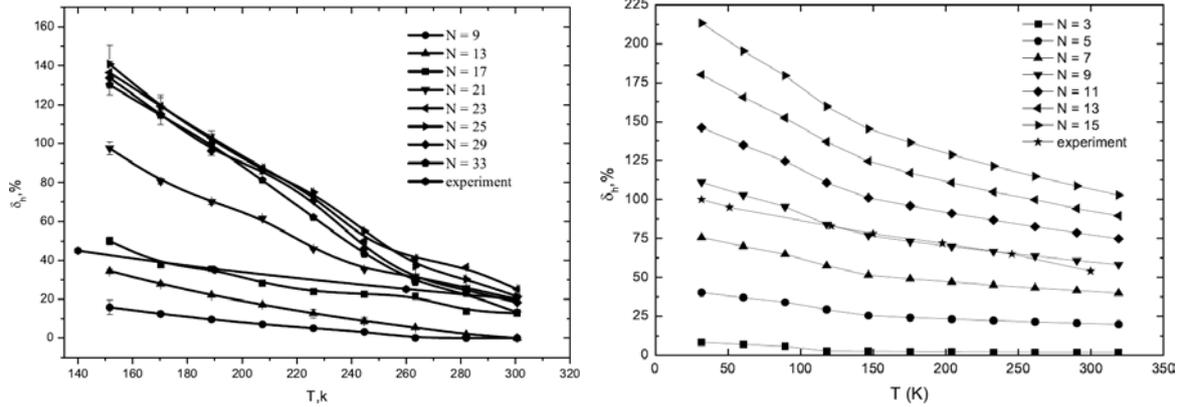


Fig. 3. The dependence of the CPP-MR of a trilayer structures Fe/Cr(100)/Fe (a) and Co/Cu(100)/Co (b) on the temperature for different values N of the thickness of ferromagnetic films. The comparison of the calculated and experimentally measured in [6] temperature dependences was made for structures with the thickness of the Fe film equal to 4 nm ($N = 21$ ML) and with the thickness of the Co film equal to 1.2 nm ($N = 9$ ML).

where $\mu_{\uparrow,\downarrow}$ is the electron mobility, ΔE_i characterizes the change of system energy connected with electron jump from i -cell to a neighbouring cell. $\Delta E_{i,\uparrow,\downarrow}$ is determined by the relation in case of CPP-MR

$$E_{i,\uparrow,\downarrow} = \mp J \left[\sum_{j \neq i} S_j^z (n_{j\uparrow} - n_{j\downarrow}) - S_i^z (n_{i\uparrow} - n_{i\downarrow}) \right], \quad (6)$$

and following relation for CIP-MR

$$E_{i,\uparrow,\downarrow} = \mp J \left[\sum_{j \neq i} S_j^z (n_{j\uparrow} - \alpha n_{j\downarrow}) - S_i^z (n_{i\uparrow} - \alpha n_{i\downarrow}) \right]. \quad (7)$$

The phenomenological parameter $0 < \alpha < 1$ is introduced in (7) which characterizes the spin flip scattering process in case of CIP geometry.

On the basis of the above presented relations, we calculated the temperature dependence of the CPP- and CIP-MR for the trilayer structure with different thicknesses N of ferromagnetic films. The procedure of calculation consists of the following steps: the first step is connected with Monte Carlo simulations of a magnetic structure in the equilibrium state at temperature T with determination of the magnetization of ferromagnetic films m_1 and m_2 , which gives the possibility of calculating the electron densities $n_{\uparrow,\downarrow}$ for film cells; in the second step the average electron velocities $\mathbf{V}_{\uparrow,\downarrow}$ and the current densities $\mathbf{J}_{\uparrow,\downarrow}$ are calculated under relations (5)–(7) subject to the spin configuration realized at a given time of the simulation and averaged over Monte Carlo steps at times of the equilibrium state simulation; in the last step the calculation of the CPP- or CIP-MR is carried out under relation (4).

Graphs of the calculated temperature dependence of the CPP-MR are presented in Figure 3 for the multilayer structures Fe/Cr(100)/Fe and Co/Cu(100)/Co with different thicknesses N of the magnetic films. The values of exchange integral was calculated using Curie-Weiss theory, $J = 1.7 \cdot 10^{-14}$ erg for Fe and $J = 4.4 \cdot 10^{-14}$ erg for Co. The magnetoresistance for the Fe/Cr(100)/Fe system is characterized by increase for films with thicknesses in the interval $N = 9 \div 25$, but the magnetoresistance begins to decrease with a further increase in the thickness. For the Co/Cu(100) system, it can be seen that the magnetoresistance increases with increasing thickness of Co film in whole considered thickness range. We carried out the comparison of the calculated and experimentally measured in [6] temperature dependences of the CPP-MR for structures with the thickness of the Fe films

equal to 4 nm, corresponding to $N = 21$ ML and with the thickness of the Co films equal to 1.2 nm, corresponding to $N = 9$ ML. One can see in Figure 3 that the calculated temperature dependence of the CPP-MR agrees very well with experimental data.

Calculation of the CIP-MR is begun at the first step from determination of the phenomenological parameter of scattering α as a value for which the best agreement of the CIP-MR with experimental results will be achieved. For the Fe/Cr(100)/Fe system, the best agreement of calculated CIP-MR with experimental data [6] is observed with $\alpha_{\text{FeCr}} = 0.36$ (see Figure 4(a)) and with $\alpha_{\text{CoCu}} = 0.20$ for Co/Cu(100)/Co system (Figure 4(b)). The results of calculation presented in Figure 4 show that the CIP-MR is decreased with increasing the parameter of scattering α .

At the second step, we calculated the CIP-MR with appointed values of α and determined the temperature dependence of the CIP-MR on thickness N of the magnetic films (Figure 5). For the Fe/Cr(100)/Fe system, the CIP-MR is characterized by increase for films with thicknesses in the interval $N = 9 \div 25$, but the CIP-MR begins to decrease with a further increase in the thickness. For the Co/Cu(100)/Cu system, the CIP-MR increases with increasing thickness N ferromagnetic film in the considered range of thicknesses. Results of our calculations demonstrate that the magnetoresistance in the case of CPP geometry is higher than the CIP-MR, that is confirmed by experimental data [6].

4 Conclusions

In this paper, we presented the basic statements of our methodology for determination of the magnetoresistance in case of measurements both with the current perpendicular to plane (CPP-MR) and with the current in plane (CIP-MR). We introduced for calculation of the CIP-MR a phenomenological parameter of electron scattering at F/N interfaces. We realized the methodology for calculation of the CPP- and CIP-MR in Fe/Cr(100)/Fe and Co/Cu(100)/Co multilayer structures. The parameter of scattering was determined from comparison of calculated and experimentally measured CIP-MR values for Fe/Cr(100)/Fe and Co/Cu(100)/Co structures. We study the temperature dependence of the CPP- and CIP-MR in

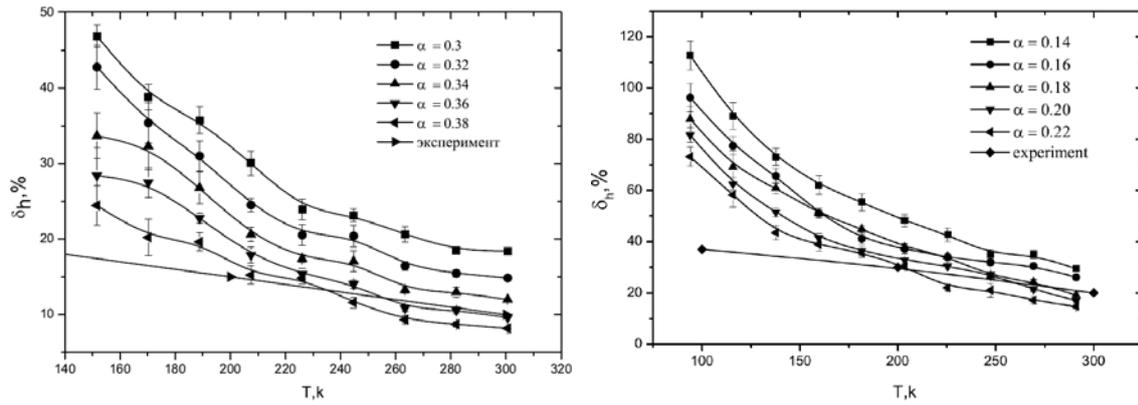


Fig. 4. The dependence of the CPP-MR of a trilayer structures Fe/Cr(100)/Fe (a) and Co/Cu(100)/Co (b) on the temperature for different values of the spin flip scattering parameter α . The comparison of the calculated and experimentally measured in [6] results was carried out with the thickness of the Fe films equal to 4 nm ($N = 21$ ML) and with the thickness of the Co films equal to 1.2 nm ($N = 9$ ML).

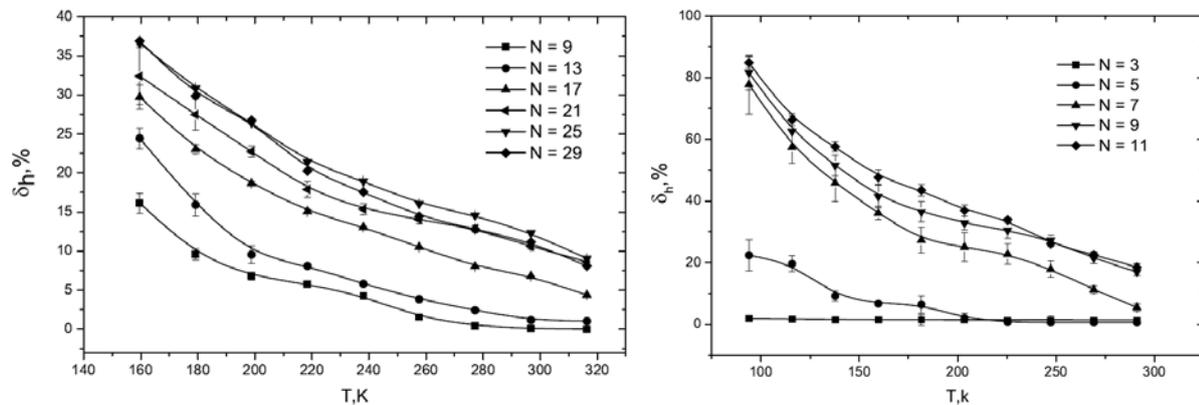


Fig. 5. The dependence of the CPP-MR of a trilayer structures Fe/Cr(100)/Fe (a) and Co/Cu(100)/Co (b) on the temperature for different values N of the thickness of ferromagnetic films.

Fe/Cr(100)/Fe and Co/Cu(100)/Co structures on thickness N of the magnetic films.

We carried out the comparison of the calculated and experimentally measured in [6] temperature dependences of the MR for these structures. It was shown that the calculated temperature dependence of the CPP- and CIP-MR agrees very well with experimental data.

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References

1. C. Chappert, A. Fert, F.N. Van Dau, Nature Mater. **6**, 813 (2007)
2. P.V. Prudnikov, V.V. Prudnikov, M. A. Medvedeva, JETP Lett. **100**, 446 (2014)
3. P.V. Prudnikov, V.V. Prudnikov, M.A. Menshikova, N.I. Piskunova, J. Magn. Magn. Mater. **387**, 77 (2015)
4. V.V. Prudnikov, P.V. Prudnikov, D.E. Romanovskii, JETP Lett. **102**, 668 (2015)
5. V.V. Prudnikov, P.V. Prudnikov, D.E. Romanovskii, J. Phys. D: Appl. Phys. **49**, 235002 (2016)
6. M.A. Gijs, S.K.J. Lenczowski, J.B. Giesbers, et al., J. Appl. Phys. **75**, 6709 (1994)
7. A. Berger, H. Hopster, Phys. Rev. Lett. **73**, 193 (1994)
8. F. Huang, M.T. Kief, G.J. Mankey, R.F. Willis, Phys. Rev. B **49**, 3962 (1994)