Influence of diffuse interfaces on the magnetoresistance in trilayer magnetic structures

Marina V. Mamonova, Vladimir V. Prudnikov, Pavel V. Prudnikov, and Anna A. Samoshilova

Omsk State University, Mira 55A, Russia
E-mail: *samoshilovaaa@stud.omsu.ru

Abstract. The numerical Monte Carlo study of influence of diffuse interfaces on the magnetoresistance in trilayer magnetic structures Co/Cu(100)/Co and Pt/Co/Cu(100)/Co/Pt is carried out. The calculations of temperature dependence of the CPP magnetoresistance are realized for structures with thickness of cobalt films N=11 monolayers for cases with sharp and diffuse interfaces. Comparison of results shows that diffuse interfaces lead to appreciable influence on the magnetoresistance in these nanostructures.

1. Introduction
Phenomena of giant magnetoresistance (GMR) are observed in trilayer nanostructures which consist of ferromagnetic films based on Fe, Co and Ni magnetic transition metals and separated by nonmagnetic films on the base of Cr, Cu, Ir metals with nanometer thicknesses[1]. Values of the magnetoresistance attaining more than 100 % at low temperatures stimulate application of such structures for creation of new generation of hard disk read heads and magnetoresistive sensors, spintronic and memory devices, etc[2].

We have developed in [3,4] the methodology for determination of the magnetoresistance for CPP geometry (the current perpendicular to plane) by the Monte Carlo method and calculated temperature dependence of the magnetoresistance for trilayer and spin-valve magnetic structures with GMR effects on different thicknesses of the ferromagnetic films. Model concepts of this methodology use an assumption of existence of sharp interfaces between ferromagnetic and nonmagnetic metal films. It is well known that quality of interfaces in magnetic nanostructures essentially affects the magnetoresistance and leads to decrease of the magnetoresistance for magnetic nanostructures with diffuse interfaces[5]. Quality of interfaces depends in a less degree on thermodynamic conditions, in which a magnetic structure is found, but depends substantially on sputtering technology.

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 nanostructures 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[6,7]. The multilayer magnetic structure Co/Cu(100)/Co extensively usable in active elements of spintronic devices is characterized by anisotropy of ”easy” magnetic plane type with magnetization oriented in plane of cobalt film. The structure Pt/Co/Cu/Co/Pt with...
cobalt films coated by ultrathin platinum films is already characterized by anisotropy of “easy” magnetic axis type with magnetization oriented perpendicularly to plane of cobalt film. As it has been shown in [8], Pt/Co bilayer possess giant energy of magnetic anisotropy and high Curie temperatures attaining 500 K in ultrathin films. Combination of high Curie temperature in cobalt films and perpendicular magnetic anisotropy generated in Pt/Co bilayer makes it possible to increase significantly magnetoresistance in Pt/Co/Cu/Co/Pt structure in comparison with Co/Cu/Co structure [9].

In this paper, we expand our methodology [3,4,10] for study of influence of diffuse interfaces between magnetic and nonmagnetic films on the magnetoresistance in trilayer magnetic structures Co/Cu(100)/Co and Pt/Co/Cu(100)/Co/Pt with different types of magnetic anisotropy.

2. Model and methods
We use the Hamiltonian of the anisotropic Heisenberg model [6,7] for the Monte Carlo statistical description of the magnetic properties of Co films for Co/Cu(100)/Co trilayer structure with the in plane magnetization in Co films in the form

\[ H = - \sum_{<i,j>} J_{ij} \left[ (S^x_i S^x_j + S^y_i S^y_j) + (1 - \Delta_1(N))S^z_i S^z_j \right] \quad (1) \]

and for Pt/Co/Cu(100)/Co/Pt structure with the out of plane magnetization in Co films in the form

\[ H = - \sum_{<i,j>} J_{ij} \left[ (1 - \Delta_2(N))(S^x_i S^x_j + S^y_i S^y_j) + S^z_i S^z_j \right] \quad (2) \]

Therein, \( J_{ij} \) characterizes the short-range exchange interaction between the spins \( S_i \), fixed at the sites of a face-centered cubic (fcc) lattice for Co films. \( S_i = (S^x_i, S^y_i, S^z_i) \) is introduced as a three-dimensional unit vector. \( \Delta_1,2(N) \) are anisotropy parameters. The dependence of the anisotropy parameters \( \Delta_{1,2}(N) \) on the film thickness \( N \) was calculated in compliance with experimental data for the critical temperatures in Ni/Cu(100), Co/Cu(100) [11] and in Ni(111)/W(110) [12] films as quantities determined by relative change of the ferromagnetic transition temperature \( T_c(N) \) in magnetic films to \( T_c(\infty) \) in the bulk samples. The resulting dependences of \( \Delta_{1,2}(N) \) are given in Fig.1.

![Figure 1](image1.png)

**Figure 1:** The dependence of the anisotropy parameters \( \Delta_1(N) \) (a) and \( \Delta_2(N) \) (b) on the thickness of the ferromagnetic film \( N \) in units of monatomic layers (ML). The squares (a) correspond to experimental data for Ni/Cu(100) and Co/Cu(100) [11], the circles (b) correspond to experimental data for Ni(111)/W(110) [12].

We consider a model for simulation of trilayer nanostructure, which consists of two ferromagnetic films separated by a nonmagnetic metal film (Fig.2). The simulations were performed for films with linear sizes \( L \times L \times N \) with applied periodic boundary conditions.
in the plane of the film. $L \times L$ gives the number of spins in each layer, and $N$ is the number of monolayers in the thin film. 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 interlayer antiferromagnetic interaction between the films is taken as $J_2 = 0.3J_1$. The temperature $T$ of the system is measured in units of the exchange integral $J_1/k_B$. The temperature scale is defined through the value of the exchange integral $J_1 = 4.4 \cdot 10^{-13}$ erg corresponding to the bulk cobalt.

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

$$\delta_h = \frac{R_{AP} - R_P}{R_P}$$

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. Calculation of the magnetoresistance was carried out for CPP geometry, when the current conduction is realized perpendicular to the layers and the electrodes are situated on both sides of the structure. Experimental study shows that the CPP magnetoresistance is characterized by larger values than the CIP magnetoresistance (the current in plane), approximately twice as high [13]. 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-MR

We present in this section the methodology which was developed for the calculation of magnetoresistance in multilayered structure in case of CPP 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 $R_P = (2R_\uparrow R_\downarrow)/(R_\uparrow + R_\downarrow)$. Consequently, the magnetoresistance of the trilayer structure is determined by the relation

$$\delta_h = \frac{(R_\uparrow - R_\downarrow)^2}{4R_\uparrow R_\downarrow} = \frac{(J_\uparrow - J_\downarrow)^2}{4J_\uparrow J_\downarrow}$$
where $J_{\uparrow \downarrow} = e n_{\uparrow \downarrow} V_{\uparrow \downarrow}$ 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 $V_{\uparrow \downarrow}$ 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 $V_{\uparrow \downarrow}$ can be expressed through the electron mobility and the external electric field intensity $E$, 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:

$$< V_{\uparrow \downarrow} > = \mu_{\uparrow \downarrow} E = \frac{e}{T} E e^{-\Delta E_{\uparrow \downarrow} / T}$$

where $\mu_{\uparrow \downarrow}$ is the electron mobility, $\Delta E_{\uparrow \downarrow}$ characterizes the change of system energy connected with electron jump from $i$-cell to a neighbouring cell. $\Delta E_{\uparrow \downarrow}$ is determined by the relation in case of Pt/Co/Cu(100)/Co/Pt structure with the out of plane magnetization

$$E_{i\uparrow \downarrow} = \mp J_{1} \left[ \sum_{j \neq i} S_{j}^{z} (n_{j \uparrow} - n_{j \downarrow}) - S_{i}^{z} (n_{i \uparrow} - n_{i \downarrow}) \right]$$

and following relation for Co/Cu(100)/Co structure with the in plane magnetization

$$E_{i\uparrow \downarrow} = \mp J_{1} \left[ \sum_{j \neq i} S_{j}^{x} (n_{j \uparrow} - n_{j \downarrow}) - S_{i}^{x} (n_{i \uparrow} - n_{i \downarrow}) \right]$$

On the basis of the above presented relations, we calculated the temperature dependence of the CPP-MR for the trilayer structures with different thicknesses $N$ of ferromagnetic films. We have used the infinitesimal small magnitude of external field $h/k_B T = g \mu_B H/k_B T << 1$ in direction of magnetic anisotropy. 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 $V_{\uparrow \downarrow}$ and the current densities $J_{\uparrow \downarrow}$ 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-MR is carried out under relation (4).

At the first stage of this study, we realize calculation of temperature dependence of the magnetoresistance $\delta(T, N)$ in Co/Cu(100)/Co structure on the thickness of the cobalt films $N$ with setting of sharp interfaces between Co and Cu films. Results of calculation are presented in Fig.3. It can be seen that the magnetoresistance increases with increasing thickness of Co film in whole considered thickness range with $N = 3 \div 15$ ML. We carried out the comparison of the calculated and experimentally measured in [13] temperature dependence of the CPP-MR for structure with the thickness of the Co films equal to 1.2 nm, corresponding to $N = 9$ ML. One can see in Fig.3 that the calculated temperature dependence of the CPP-MR agrees very well with experimental data.

Results of calculation of the CPP-MR $\delta(T, N)$ in Pt/Co/Cu(100)/Co/Pt structure are given in Fig.4. Comparison of $\delta(T, N)$ in Fig.3 and Fig.4 shows that change of magnetic anisotropy orientation from parallel to perpendicular to plane of ferromagnetic film leads to significant increase of magnetoresistance especially for structures with small thicknesses of the cobalt
Figure 3: The dependence of the CPP-MR $\delta(T,N)$ in tri-layer Co/Cu(100)/Co structure on the temperature for different thicknesses $N$ of the cobalt films. The comparison of the calculated and experimentally measured in [13] temperature dependences was made for structure with the thickness of the Co film equal to 1.2 nm ($N=9$ ML).

Figure 4: The dependence of the CPP-MR $\delta(T,N)$ in trilayer Pt/Co/Cu(100)/Co/Pt structure on the temperature for different thicknesses $N$ of the cobalt films.

films. In addition, influence of anisotropy reorientation on the magnetoresistance is reduced with increase of ferromagnetic film thickness.

At sequent stage, we introduce a model with diffuse interfaces for Co/Cu(100)/Co and Pt/Co/Cu(100)/Co/Pt structures with thickness of Co films $N=11$ ML. Scheme of ionic planes arrangement in Co and Cu films parallel to Cu face (100) is given in Fig.5. Diffuse interface effects for fcc-lattices of Co and Cu films are represented as mutual partial replacement of Cu ions in planes $N_{Cu}=1,2$ by Co ions from planes $N_{Co}=10$ and $N_{Co}=11$. Consequently, a diluted magnetic matter with quenched defects is introduced in interfaces of structure, when a random position of atoms is not changed over time interval of measurement of characteristics. For description of Co ions distribution in two surface planes of Co film and two surface planes of Cu film, there are introduced the values of spin concentration $p_{10Co}=0.75$ and $p_{11Co}=0.5$ for ionic planes of Co film with $N_{Co}=10,11$ and $p_{2Cu}=0.5$ and $p_{2Cu}=0.25$ for ionic planes of Cu film with $N_{Cu}=1,2$ in accordance with images given in Fig.5. We must note that spin concentrations in our model of diffuse interfaces with smearing effects affecting on two surface monolayers only exceeds the threshold of spin percolation.

Figure 5: Model of Co/Cu(100)/Co structure with diffused interfaces between Co film (on the left) and Cu film (on the right). Full circles correspond to Co and open circles to Cu.

On the base of this model, we have calculated by the Monte Carlo method the temperature dependence of the CPP magnetoresistance $\delta(T)$ in Co/Cu(100)/Co and Pt/Co/Cu(100)/Co/Pt
structures with diffuse interfaces on the assumption of temperature influence neglecting on degree of smearing of interfaces. We considered cases with different mean free paths of electron in ferromagnetic films, when mean free paths of electron are equal to thickness $N=11$ ML and to $N=13$ ML. Calculation of the magnetoresistance was realized after systems relaxation during 20 000 MCS/s and averaged after that on 20 000 MCS/s. Results of calculation are presented in Fig.6 and Fig.7, consequently.

Figure 6: Temperature dependence of the magnetoresistance $\delta(T)$ in Co/Cu(100)/Co (a) and Pt/Co/Cu(100)/Co/Pt (b) structures with thickness of Co films $N=11$ ML (curve 1) and $N=13$ ML (curve 2) in case with sharp interfaces and structures with $N=11$ ML (curve 3) in case with diffuse interfaces and with mean free path of electron equal to thickness $N=11$ ML.

Comparison of obtained values of the magnetoresistance $\delta(T)$ in Fig.6 for structures with sharp and diffuse interfaces shows that the presence of diffuse interfaces leads to decrease of the magnetoresistance in low temperature range with respect to structures with sharp interfaces and thickness $N=11$ ML of cobalt films. This decrease of the magnetoresistance $\delta(T)$ is weaker in Co/Cu(100)/Co structure and developed in lower temperature range with $T < 125$ K than in Pt/Co/Cu(100)/Co/Pt structure where decrease of $\delta(T)$ is predicted for $T < 180$ K. The magnetoresistance $\delta(T)$ in structures with sharp and diffuse interfaces demonstrates close values in higher temperature range in relatively to noted temperatures.

The case with mean free paths of electron equal to thickness $N=13$ ML and given in Fig.7 shows some peculiarities. So, the curves of temperature dependence of the magnetoresistance $\delta(T)$ in Co/Cu(100)/Co structure with sharp ($N=11$ ML) and diffuse interfaces are intersected at temperature $T^* \approx 250$ K. For temperatures $T < T^*$, the $\delta(T)$ in structure with diffuse interfaces exceeds the $\delta(T)$ in structure with sharp interfaces and comes nearer to the magnetoresistance in structure with thickness of Co films $N = 13$ ML. In case with higher temperatures $T > T^*$, the magnetoresistance $\delta(T)$ in structure with diffuse interfaces is reduced with increase of temperature in comparison with the $\delta(T)$ in structure with sharp interfaces and $N = 11$ ML. The magnetoresistance $\delta(T)$ in Pt/Co/Cu(100)/Co/Pt structure demonstrate different dependence. So, the presence of diffuse interfaces leads to decrease of the magnetoresistance $\delta(T)$ in low temperature range for $T < 180$ K with respect to structure with sharp interfaces and thickness $N = 13$ ML of cobalt films, but with values $\delta(T)$ are higher than in structure with sharp interfaces and thickness $N = 11$ ML. For temperature range with $T > 180$ K, the magnetoresistance $\delta(T)$ in structures with sharp ($N=13$ ML) and diffuse interfaces demonstrates close values.
Figure 7: Temperature dependence of the magnetoresistance $\delta(T)$ in Co/Cu(100)/Co (a) and Pt/Co/Cu(100)/Co/Pt (b) structures with thickness of Co films $N=11$ ML (curve 1) and $N=13$ ML (curve 2) in case with sharp interfaces and structures with $N=11$ ML (curve 3) in case with diffuse interfaces and with mean free path of electron equal to thickness $N=13$ ML.

4. Conclusions
In this paper, we have studied an influence of diffuse interfaces on the magnetoresistance in trilayer magnetic structures Co/Cu(100)/Co and Pt/Co/Cu(100)/Co/Pt with different types of magnetic anisotropy. We presented results of calculation of temperature dependence of the CPP magnetoresistance $\delta(T,N)$ in these structures with sharp interfaces for different thicknesses $N$ of ferromagnetic films. It has been shown that change of magnetic anisotropy orientation from parallel to plane of ferromagnetic film in Co/Cu(100)/Co structure to perpendicular to plane in Pt/Co/Cu(100)/Co/Pt structure leads to significant increase of the magnetoresistance. We have introduced a model of diffuse interfaces as diluted magnetic interlayers with quenched Co atoms and calculated the CPP magnetoresistance for cases with different mean free paths of electron in ferromagnetic films, when free paths of electron are equal to thickness of ferromagnetic film and exceed the thickness of ferromagnetic film on interface smearing size. In first case, it has been revealed that presence of diffuse interfaces leads to decrease of the magnetoresistance in low temperature range with respect to structures with sharp interfaces, but it leads to close values of the magnetoresistance in high temperature range. In second case, we revealed the similar temperature dependence of the magnetoresistance, but with larger values determined by thickness of ferromagnetic film with subject to interface smearing size.

Thereby, results of our study demonstrate that diffuse interfaces lead to appreciable influence on the magnetoresistance in nanostructures which depends on degree of interfaces smearing, type of magnetic anisotropy in ferromagnetic films and adequacy of mean free paths of electron in ferromagnetic film with thickness of this film with subject to interface smearing size. Considered phenomenon is a result of simultaneous influence of conduction electrons scattering on quenched magnetic impurities quenched in interface and changes in the boundary conditions for conduction electrons.

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References

[1] Fert A 2008 Phys. Usp. 51 1336; Grunberg P A 2008 Phys. Usp. 51 1349
[2] Prinz G A 1999 J. Magn. Magn. Mater. 200 57
[3] Prudnikov V V, Prudnikov P V and Romanovskii D E 2015 JETP Lett. 102 668
[4] Prudnikov V V, Prudnikov P V and Romanovskii D E 2016 J. Phys. D: Appl. Phys. 49 235002
[5] Chuprakov S A et al 2018 Phys. Met. Metallogr. 119 309
[6] Prudnikov P V, Prudnikov V V and Medvedeva M A 2014 JETP Lett. 100 446
[7] Prudnikov P V, Prudnikov V V, Menshikova M A and Piskunova N I 2015 J. Magn. Magn. Mater. 387 77
[8] Morgunov R et al 2017 Superlattices Microstruct. 104 50
[9] Prudnikov P V, Prudnikov V V, Mamonova M V and Piskunova N I 2019 J. Magn. Magn. Mater. 482 201
[10] Romanovskii D E, Mamonova M V, Prudnikov V V and Prudnikov P V 2017 SibFU J. Math. Phys. 10 65
[11] Huang F, Kief M T, Mankey G J and Willis R F 1994 Phys. Rev. B 49 3962
[12] Li Y and Baberschke K 1992 Phys. Rev. Lett. 68 1208
[13] Gijs M A et al 1994 J. Appl. Phys. 75 6709