

# First-principle calculations of the exchange interaction characteristics for multilayer magnetic structures

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**Abstract.** Magnetic multilayer structures which consist of the ferromagnetic layers separated by nonmagnetic layers with giant magnetoresistance (GMR) are widely used as spintronic devices and read heads of hard disks. In this work magnetic and exchange interaction characteristics of Co/Cu/Co, Ni/Cu/Ni and Fe/Cr/Fe multilayer structures are studied by using VASP software package within the Projector Augmented Wave (PAW) method with generalized-gradient approximation (GGA PBE). The finite temperature magnetism of these structures was studied by Monte-Carlo simulations with the use of the exchange interaction parameters obtained from the ab initio results.

## 1 Introduction

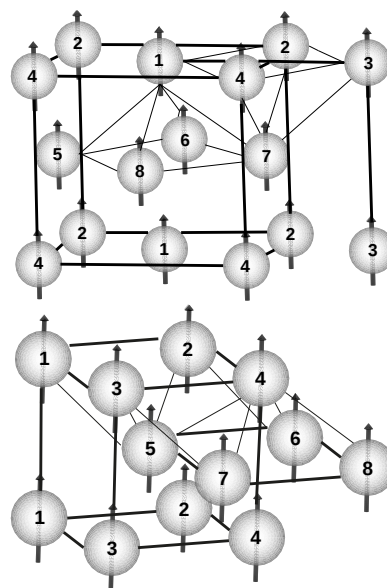
The ultrathin films on the basis of the magnetic transition metals are used as a components for magnetic multilayer structures with giant magnetoresistance(GMR) which consist of the ferromagnetic layers separated by nonmagnetic layers [1]. These magnetic structures are widely used as read heads of hard disks, memory and spintronic devices [2]. At present, the development of modern computer technology and methods for solving large systems of equations makes it possible to obtain with high accuracy in the calculation of the properties of substances from the first principles of the characteristics of low-dimensional systems that are difficult or expensive to investigate in an experiment. The first-principles calculations of the electronic and crystal structure of magnetic materials are based on the spin theory of the density functional and the numerical solution of the system of Kohn-Sham equations. In this paper atomic structures, magnetic properties and exchange interaction characteristics of ferromagnetic films on Cu and Cr substrates are studied with the use of VASP (Vienna Ab-Initio Simulation Package) software package [3].

## 2 Model and methods

The layers of ferromagnetic atoms in systems Co/Cu/Co, Ni/Cu/Ni and Fe/Cr/Fe are placed pseudomorphically on each side of the nonmagnetic slab to retain the inversion symmetry. The magnetic moment of atoms is directed collinearly along the *z* axis. The substrate with 100 orientation surface plane is modeled by the three-layer slab. Supercells for BCC (Fe/Cr)and FCC(Ni/Cu and Co/Cu) systems are given in Fig. 1. We modeled the surface cell

using an one atom in monolayer to calculate the energy of film formation and four atoms in a monolayer to calculate the exchange integrals.

We carried out calculations with the use of VASP by means of the Projector Augmented Wave (PAW) method with PBE [4] approximation to describe the exchange-correlation interactions. We calculated the optimized lat-



**Figure 1.** Atoms configurations in FCC and BCC super cells for three monolayers film. The arrows represent magnetic spins directions. The lines show connections the nearest and next-nearest neighbors atoms.

tice constant for bulk Cu through local density approximation (LDA)  $a = 3.524(1)\text{\AA}$  and generalized gradient approximation (GGA)  $a = 3.6367(5)$  calculations, that cor-

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**Table 1.** Results of calculation of the total  $E_{\text{tot}}$  and film formation  $E_{\text{film}}$  energies and magnetic moment  $\mu_{\text{tot}}$ .

Position	$E_{\text{tot}}, \text{eV}$	$E_{\text{film}}, \text{eV}$	$\mu_{\text{tot}}, \frac{\mu_B}{\text{at}}$
Ni/Cu(100)fcc	-27.588	-1.405	0.330
Ni/Cu(111)fcc	-28.118	-1.159	0.430
Ni/Cu(111)bridge	-28.042	-1.120	0.454
Ni/Cu(111)ontop	-27.347	-0.774	0.531

responds to the value  $a = 3.6369 \text{ \AA}$  obtained by other authors [5]. Also, the application of GGA approach for magnetic calculations is preferable due to more accurate band calculations and further accurate calculations of magnetic moments.

To determine the Ni film formation energy, it is necessary to calculate the difference between total energy of the system and the energy of its components:

$$E_{\text{film}} = \frac{1}{2n}(E_{\text{NiCu}} - E_{\text{Cu}} - 2nE_{\text{Ni}}), \quad (1)$$

where  $E_{\text{Cu}}$  is the total energy of 5-ML Cu slab;  $E_{\text{NiCu}}$  is the total energy of Ni/Cu/Ni system;  $E_{\text{Ni}}$  is the total energy of 1-ML Ni slab;  $n$  is Ni film thickness in units of monolayers (we used one atom into the monolayer).

We obtained the energy of the film formation for Ni/Cu(100)/Ni system and the magnetic moment atom in 1-ML Ni slab as the functions of convergence parameters. We confined ourselves to values of the plane waves cut-off energy  $E_{\text{max}} = 350 \text{ eV}$  and Monkhorst Pack grid size  $11 \times 11 \times 1$ . Magnetic moments  $\mu = 1.02(7)\mu_B$  and  $\mu = 0.33(4)\mu_B$ , which were calculated correspondingly for atom free standing monolayer Ni film and for atom in 1-ML Ni on Cu(001), are in good agreement with results  $\mu = 0.95\mu_B$  and  $\mu = 0.37\mu_B$  obtained by other authors[6].

Results of calculation of the total and film formation energies, interlayer distance relaxation parameters and magnetic moments are given in table 1. Comparison of the calculated film formation energies for various Ni atom positions (ontop, bridge, fcc) on Cu(111) substrate shows that more energetically favorable position is the position of repeating structure of the substrate. This position of the magnetic atoms are used in further calculations.

We considered the possibility of realization of the Cu/Ni/Cu(001) "sandwich" structure with two additional Cu cap layers, which are placed pseudomorphically on each side of the Ni/Cu(001) slab. The calculations show that the energy of monolayer film system  $E_{\text{tot}} = -27.134 \text{ eV}$  is greater than in the case of formation of the sandwich structure  $E_{\text{tot}} = -28.287 \text{ eV}$ . Therefore, these results determine that the formation of a sandwich structure is energetically more favorable.

The magnetic moment is the most fundamental quantity in magnetism and yet very difficult to measure experimentally in the case of thin films. The calculated values of the magnetic moments atoms at film layers and 1-st substrate layer for Co/Cu/Co, Ni/Cu/Ni and Fe/Cr/Fe multilayer structures are presented in table 2.

Comparison of the magnetic moments of the atoms in different layers allows to conclude that the atoms most distant from the substrate have greatest magnetic moment.

**Table 2.** The calculated values of the  $\mu_0$  – magnetic moment atom at 1-st substrate layer;  $\mu_i$  – magnetic moment atom at  $i$  film layer;  $\mu_{\text{tot}}$  – average magnetic moment.

	$\mu_0$	$\mu_1$	$\mu_2$	$\mu_3$	$\mu_{\text{tot}}$
	$\mu_B/\text{at}$	$\mu_B/\text{at}$	$\mu_B/\text{at}$	$\mu_B/\text{at}$	$\mu_B/\text{at}$
Ni/Cu/Ni	0.014	0.489	0.678	0.776	0.622
[7]		0.51	0.71	0.81	
[8]		0.3(1)	0.6(1)	0.8(1)	
Co/Cu/Co	0.024	1.602	1.580	1.825	1.670
Fe/Cr/Fe	-0.318	2.084	2.417	2.932	2.349

This regularity was also established both in experimental [8] and theoretical [7] investigations. Also, we can see in table 2 that the surface atoms of the nonmagnetic substrate are magnetized, and the directions of the magnetic moments for iron and chromium atoms are opposite in the Fe / Cr / Fe system.

### 3 Methodology and results of calculation exchange interaction parameters

The energy of quantum Heisenberg magnet per unit cell can be written as

$$H = -\frac{1}{2n} \sum_{i,j} J_{ij} S_i S_j, \quad (2)$$

where the summations are over the all sites in the unit cell,  $S_i$  are quantum spin operators,  $n$  is the number of unit cells in the crystal. The exchange interaction parameters of nearest neighbors and the next-nearest neighbors atoms ( $d_1 = (a\sqrt{2})/2$  and  $d_2 = a$  for FCC structure as it is shown in Fig. 1) can be obtained from the difference of the total energy for the ferromagnetic and antiferromagnetic configurations of spins in the film:

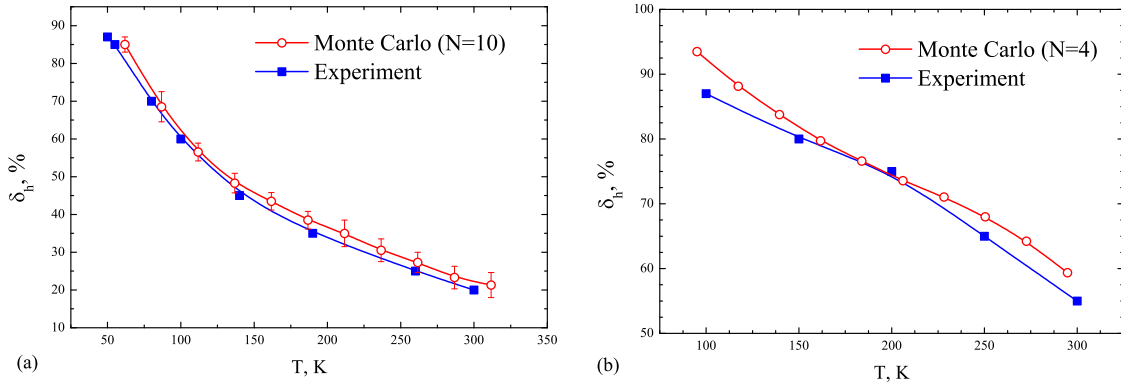
$$N_{ij} J_j = \Delta E_i = E_i^{\text{AFM}} - E^{\text{FM}}, \quad (3)$$

where  $N_{ij}$  is a number of antiparallel pairs in one unit cell in the  $i$ -th AFM state for nearest neighbors ( $j = 1$ ) and the next-nearest neighbors ( $j = 2$ ) atoms. The values of parameters in this equation, obtained by our calculations are given in table 3–4. The considered antiferromagnetic configurations of spins are given in table 3. The sign '+' indicates the direction of the spin projection - upwards, the sign '-' the direction down. The order of alternation of signs corresponds to the numbering of atoms, an example of which is shown in Fig 1.

The investigation calculated values of the total energies for the ferromagnetic EF and antiferromagnetic EAF spin configurations of multilayer systems (Table 4) shows that, regardless of the system, a fully ordered ferromagnetic state is energetically more favorable.

### 4 Results of calculations of the magnetoresistance

On the basis of these values of the exchange interaction integrals, we calculated the temperature dependence of the



**Figure 2.** Comparison of the calculated and experimentally measured [1] temperature dependence of the magnetoresistance with the use of the ab initio determined values of the exchange integral for Fe/Cr/Fe (a) and Co/Cu/Co (b) structures.

**Table 3.** Antiferromagnetic spin configurations, the number of antiparallel pairs  $N_{ij}$ , and results of calculation of the  $i$  AFM states total energy  $EAF_i$ .

AFM state		$N_1$	$N_2$
BCC	1	20	24
	2	24	12
FCC	1	22	0
	2	18	6

**Table 4.** The calculated values of the total energies for the ferromagnetic EF and antiferromagnetic EAF spin configurations.

	EF eV	EAF1 eV	EAF2 eV
Ni/Cu/Ni	-167.819	-166.749	-166.691
Co/Cu/Co	-201.463	-197.313	-197.313
Fe/Cr/Fe	-300.036	-295.483	-295.621

**Table 5.** The calculated values of the exchange integrals of nearest neighbor and the next nearest neighbor interaction.

	$J_1 * 10^{-14}$ , erg	$J_2 * 10^{-14}$ , erg
Ni/Cu/Ni	0.65	0.56
Co/Cu/Co	2.52	1.68
Fe/Cr/Fe	1.73	0.73

magnetoresistance using the Monte-Carlo simulations for the trilayer structures Fe/Cr(100)/Fe and Co/Cu(100)/Co with different thicknesses  $N$  of ferromagnetic films. Magnetoresistance for a multilayer structures is introduced as  $\delta_h = (R_{AP} - R_P)/R_P$ , where  $R_{AP}$  and  $R_P$  are the resistance

of the structure when the magnetizations of adjacent ferromagnetic layers are aligned antiparallel and parallel orientation of the magnetization of ferromagnetic layers respectively. 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  $V$  and the current densities  $J_{i,\uparrow\downarrow} = eVn_{\uparrow\downarrow}$  are calculated under relations

$$V = \mu E = \frac{eZa^2}{kT} e^{-\frac{\Delta E_i}{kT}} E \quad (4)$$

$$E_{i,\uparrow\downarrow} = \mp J_1 \left[ \sum_{j \neq i} S_j^z (n_{j,\uparrow} - n_{j,\downarrow}) + S_i^z (n_{i,\uparrow} - n_{i,\downarrow}) \right], \quad (5)$$

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 magnetoresistance is carried out under relation  $\delta_h = \frac{(J_{\uparrow} - J_{\downarrow})^2}{4J_{\uparrow}J_{\downarrow}}$ .

In Monte Carlo calculations the temperature scale is determined through the value of the exchange integral. So for comparison of the calculated and experimentally measured temperature dependence of the magnetoresistance we used the ab initio determined values of the exchange integral.

More detailed description of Monte-Carlo simulations is presented in our papers [9, 10]. The graphs of calculated temperature dependence of the magnetoresistance are given in Fig. 2, which demonstrate a good agreement with experimental data [1].

## 5 Conclusions

In this paper, magnetic properties of Ni/Cu/Ni Co/Cu/Co and Fe/Cr/Fe trilayer structures was investigated by ab-initio methods. The exchange interaction integrals for these structures were first calculated, that allowed us to obtain the temperature dependence of the magnetoresistance,

which demonstrate a good agreement with experimental data.

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