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First-Principles Investigations of the Atomic Structure and Magnetic Properties of Ni and Co Films on Cu Substrate

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Abstract—Paper considers magnetic properties of the transition metals at nanoscale level, the total energies of the several collinear spin-configurations are calculated by using VASP software package. Energy of the film formation and the magnetic moment values were obtained for trilayer structures Ni/Cu(001)/Ni, Ni/Cu(111)/Ni and Co/Cu(001)/Co as a function of the convergence parameters and taking into account the relaxation effects, and magnetic film thickness. An influence of various Ni atom positions (ontop, bridge, fcc) and additional Cu cap layers on Ni/Cu/Ni system total energy was investigated. The exchange interaction parameters for Co/Cu(001)/Co and Fe/Cr(001)/Fe structures were calculated within a classical Heisenberg model. 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.

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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]. In this paper atomic structures and magnetic properties of ferromagnetic films on Cu substrate are studied with the use of VASP (Vienna Ab-Initio Simulation Package) software package [3] by means of the Projector Augmented Wave (PAW) method with PBE [4] version of generalized gradient approximation (GGA) to describe the exchange-correlation interactions. We obtained the optimized lattice constant for bulk Cu through LDA $a = 3.524(1)$ Åand GGA $a = 3.6367(5)$ calculations. Comparison these calculated values with the results of other authors which give $a = 3.6369$ Å [5] shows that we must use the GGA approximation for description of Ni/Cu system.

1. INVESTIGATION OF Ni/Cu(001)/Ni AND Ni/Cu(111)/Ni SYSTEMS

The layers of Ni atoms in Ni/Cu(001)/Ni and Ni/Cu(111)/Ni systems are placed pseudomorphically on each side of the slab to retain the inversion symmetry. The magnetic moment of atoms is directed collinearly along the z axis. The Cu substrate is modeled by the five-layer slab. Supercells for these systems are given in Fig. 1.

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: $E_{\text{film}} = \frac{1}{2n}\left(E_{NiCu} - E_{Cu} - 2nE_{Ni}\right)$, where E_{Cu} is the total energy of 5-ML Cu slab; E_{NiCu} is the total energy of Ni/Cu/Ni system; E_{Ni} is the total energy of 1-ML Ni slab; n is Ni film thickness in units of monolayers. We obtained the energy

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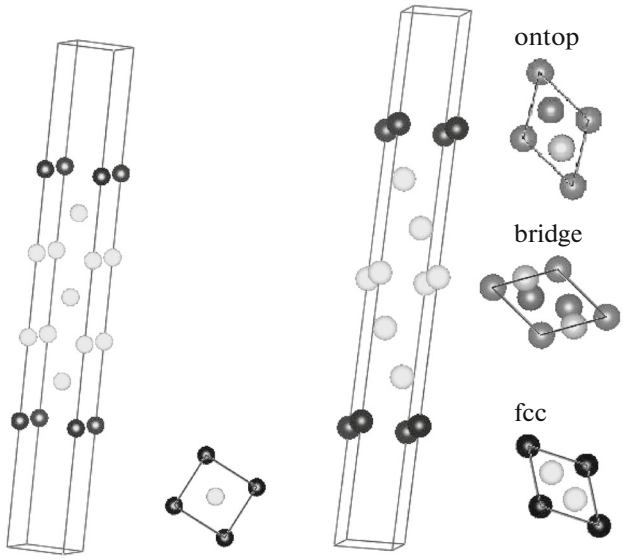

Fig. 1. The supercell structure and surface unit cell of the Ni/Cu(001) (left side) and Ni/Cu(111) (right side) systems.

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 $E_{\max} = 350$ 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 parametes 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 fcc structure of the copper.

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 $E_{\text{tot}} = -27.134$ eV is greater than in the case of formation of the sandwich structure $E_{\text{tot}} = -28.287$ eV. Therefore, these results determines that the formation of a sandwich structure is energetically more favorable. We investigated the dependence of the energy and magnetic characteristics for system Ni/Cu(100) on thickness of the Ni magnetic film from $N = 1$ to $N = 4$ monolayers. The strong increase of the film formation energy for film thickness $N = 2$ in comparison with energy for the monatomic film was established and results of calculation are demonstrated in Table 2.

2. CALCULATIONS OF THE EXCHANGE INTERACTION PARAMETERS

The energy of quantum Heisenberg magnet per unit cell can be written as $H = -\frac{1}{2n}\sum_{i,j} J_{ij} S_i S_j$, where the summations are over the all sites in the unit cell, S_i are quantum spin operators, n is the

Table 1. Results of calculation of the total E_{tot} and film formation E_{film} energies, interlayer distance relaxation parametes δ and magnetic moment μ_{tot}

Position	E_{tot}, eV	E_{film}, eV	δ_{Ni}, %	δ_{Cu}, %	μ_{tot}, $\frac{\mu_b}{\text{a}}$
Ni/Cu(100)fcc	−27.588	−1.405	−4.950	2.062	0.330
Ni/Cu(111)fcc	−28.118	−1.159	3.240	1.431	0.430
Ni/Cu(111)bridge	−28.042	−1.120	2.968	3.203	0.454
Ni/Cu(111)ontop	−27.347	−0.774	11.261	0.191	0.531

Table 2. The dependence of the film formation energy and magnetic moment on the Ni film thickness

Thickness N, ml	E_{film}, eV	μ_{tot}, μ_{B}/at
1	−1.178	0.33
2	−0.618	0.28
3	−1.703	0.55
4	−1.730	0.55

Table 3. Antiferromagnetic spin configurations, the number of antiparallel pairs N_{ij}, and results of calculation of total energy differences ΔE for 2-ML and 3-ML Co film

ith AFM state		ΔE_i, eV/at	N_{i1}	N_{i2}
1	+ − + − − + − +	0.171	13	0
2	+ + − − − − + +	0.171	8	4
1	+ − + − − + − + + − + −	0.173	22	0
2	+ + − − − − + + + + − −	0.173	18	6

Table 4. Results of calculation of the magnetic moments μ_i in the ith layer and the exchange interaction integrals for 2-ML and 3-ML Co film

	μ_1 μ_{B}/at	μ_2 μ_{B}/at	μ_3 μ_{B}/at	μ_{tot} μ_{B}/at	$J_1 \times 10^{-14}$, erg	$J_2 \times 10^{-14}$, erg
2-ML Co	1.545	1.746		1.650	4.22	5.24
3-ML Co	1.602	1.580	1.825	1.670	2.52	1.68

number of unit cells in the crystal. The crystal structure of Co/Cu/Co superlattice used here is fcc lattice structure with the doubled unit cell in the (100) surface plane and the distances between the of nearest neighbors $d_1 = (a\sqrt{2})/2$ and the next-nearest neighbors atoms $d_2 = a$. The exchange interaction parameters of nearest neighbors J_1 and the next-nearest neighbors atoms J_2 can be obtained from the difference of the total energy for the ferromagnetic and antiferromagnetic configurations of spins in the film $N_{ij}J_j = \Delta E_i = E_i^{\text{AFM}} - E^{\text{FM}}$, 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 for system consisting of two Co films with 2 and 3 monolayer thickness and separated by 3 monolayer thickness film of Cu(100), are given in Table 3.

Comparison of the magnetic moments of the atoms in different layers, which values are presented in Table 4, allows to conclude that the atoms most distant from the substrate have greatest magnetic moment. So, we can see that the increasing of the Co film thickness leads to decrease in the exchange integral. The similar calculations were realized for structure Fe/Cr(100)/Fe consisting of two ferromagnetic films of Fe(100) with 3 ML thickness separated by non-magnetic 3 ML Cr(100) film. We determined the values of the exchange interaction integral $J_1 = 1.73 \times 10^{-14}$ erg for the nearest neighbours atoms and $J_2 = 0.73 \times 10^{-14}$ erg for the next-nearest neighbours atoms. On the basis of these values of the exchange interaction integrals, we calculated the temperature dependence of the

Table 5. Comparison of the calculated δ_h and experimentally measured [1] $\delta_h^{\exp}$ temperature dependence of the magnetoresistance with the use of the ab initio determined values of the exchange integral for Co/Cu/Co and Fe/Cr/Fe structures

T, K	$\delta_h^{\exp}$, %	δ_h, %	T	$\delta_h^{\exp}$, %	δ_h, %
100	87	92.6	100	60	60.4
150	80	82.0	140	45	47.7
200	75	75.0	190	35	37.8
250	65	68.5	260	25	27.5
300	55	58.0	300	20	22.2

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. More detailed description of Monte Carlo simulations is presented in our papers [7, 8]. The results of calculation of temperature dependence of the magnetoresistance are given in in Table 5, which demonstrate a good agreement with experimental data [1].

In summary, magnetic properties of Ni/Cu/Ni and Co/Cu/Co trilayer structures as a function of the film thickness and various adatom positions was investigated by ab initio methods. The exchange interaction integrals for Co/Cu(001)/Co and Fe/Cr(001)/Fe structures were first calculated, that allowed us to obtain the temperature dependence of the magnetoresistance.

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REFERENCES

1. J. Bass and W. P. Pratt, "Current-perpendicular (CPP) magnetoresistance in magnetic metallic multilayers," J. Magn. Magn. Mater. **200**, 274–289 (1999).
2. S. N. Piramanayagam and T. C. Chong, *Developments in Data Storage: Materials Perspective* (Wiley-IEEE, New York, 2011).
3. P. G. Kresse and J. Furthmuller, "Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set," Phys. Rev. B **54**, 11169 (1996).
4. J. P. Perdew, K. Burke, and M. Ernzerhof, "Generalized gradient approximation made simple," Phys. Rev. Lett. **77**, 3865 (1996).
5. K. Lejaeghere, V. van Speybroeck, G. van Oost, and S. Cottenier, "Error estimates for solid-state density-functional theory predictions: an overview by means of the ground-state elemental crystals," Crit. Rev. Solid State Mater. Sci. **39** (1), 1–24 (2014).
6. C. S. Wang and A. J. Freeman, "Surface states, surface magnetization, and electron-spin polarization: Ni(001)," Phys. Rev. B **21**, 4585 (1980).
7. V. V. Prudnikov, P. V. Prudnikov, and D. E. Romanovskiy, "Monte Carlo simulation of multilayer magnetic structures and calculation of the magnetoresistance coefficient," JETP Lett. **102**, 668–673 (2015).
8. V. V. Prudnikov, P. V. Prudnikov, and D. E. Romanovskiy, "Monte Carlo calculations of the magnetoresistance in magnetic multilayer structures with giant magnetoresistance effects," J. Phys. D: Appl. Phys. **49**, 235002 (2016).