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Study of Magnetic Anisotropy of Cobalt Films Separated by a Copper Layer Depending on the Thickness of the Layers

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Abstract. This work is devoted to the numerical study of the magnetic properties of the Co/Cu/Co system using the VASP software package. The influence of the contributions of magnetocrystalline anisotropy and shape anisotropy on the magnetic anisotropy energy was investigated. The dependence of the magnetic anisotropy, spin-orbit interaction, and dipole-dipole interaction energies on the thickness of the magnetic layer of cobalt was obtained.

Keywords: magnetic anisotropy, ultrathin magnetic films, spin-density functional theory.

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Introduction

Thin film magnetism is an active area of research with a particular impact on technological progress. Such materials are widely used in spintronics, nanoelectronics, and microelectronics devices. For numerical Monte Carlo simulation [1] and comparison of the obtained results with experiment, it is necessary to know the value of the anisotropy parameter. For structures based on ultrathin magnetic films, the mutual orientation of magnetic moments of different layers depends on the distance between them, therefore it is possible to calculate and predict at what thickness of the nonmagnetic layer the structural configuration will be more energetically favorable. Calculations of the structure at different directions of magnetic moments (in the film plane or perpendicular to it) give us knowledge about the magnitude and type of magnetic anisotropy, which is one of the most important physical properties affecting the magnetic microstructure, remagnetization processes, and other magnetic properties [2].

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1. Model and methods

In this study, calculations were performed using the density functional theory (DFT) with the projector-augmented wave (PAW) method and the Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation. The Co/Cu/Co system was considered, with the following parameters set: the number of k-points (kpoints) was 24×24×1, and the energy cutoff (encut) parameter was set at 600 eV.

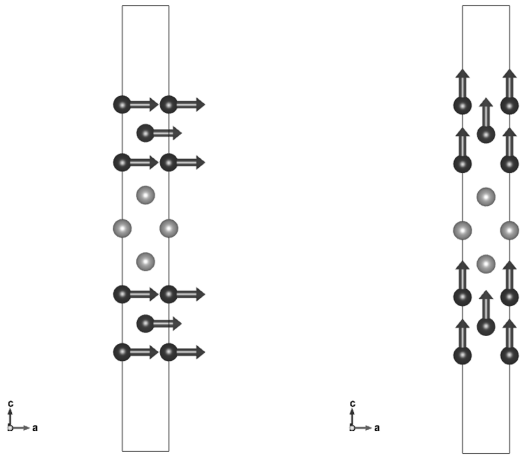

Fig. 1. The crystal structure of the Co/Cu/Co system with different orientations of the magnetic moments of the atoms

Fig. 1 shows the lattice arrangement in the Co/Cu/Co system with different orientations of the magnetic moments of the constituent atoms. The direction of the magnetic moments can influence the type of anisotropy of the system.

It is important to know the value of the magnetic anisotropy parameter as it is part of the Hamiltonian of the system with anisotropy.

$$H_{\parallel} = -\sum_{i,j} J_{i,j} \left\{ S_i^x S_j^x + S_i^y S_j^y + \left(1 - \Delta_{\parallel}\right) S_i^z S_j^z \right\}. \tag{1}$$

Let us find the dependence of the delta parameter $\Delta_{\parallel}$- the magnetic anisotropy parameter on the number of layers of the magnetic material of cobalt.

Suppose that all spins are directed along the x-axis, then $\mathrm{S_i^x} = \mathrm{S_j^x} = \mathrm{S}$; $\mathrm{S_i^y} = \mathrm{S_j^y} = 0$; $S_i^Z = S_j^Z = 0$. Let's substitute these values into (1) and get:

$$E_{\parallel} = -\sum_{i,j} J_{i,j} S^2. \tag{2}$$

Now let us direct the spins along the z-axis and, having done the same steps, we obtain:

$$E_{\perp} = -\sum_{i,j} J_{i,j} S^2 \left(1 - \Delta_{\parallel}\right). \tag{3}$$

The anisotropy parameter is therefore given by

$$\mathrm{E}_{\parallel} < \mathrm{E}_{\perp} \Rightarrow \Delta_{\parallel} = \frac{\mathrm{E}_{\parallel} - \mathrm{E}_{\perp}}{\mathrm{E}_{\parallel}}. \tag{4}$$

The magnetic anisotropy energy $E_{MA} = E_{\perp} - E_{\parallel}$ can be defined as the difference of the total energies of the system at the direction of the magnetic moments in the film plane $E_{||}$ and perpendicular to it $E_{\perp}$.

The magnetic anisotropy energy can be divided into two contributions: $E_{MA} = E_{MKA} + \Delta E_{dd}$, one of which is the magnetocrystalline anisotropy energy $E_{MKA} = \Delta E_{SOC}$ induced by spin-orbit coupling, and the other is the shape anisotropy energy ΔE_{dd} due to magnetic dipole interactions [3]. The shape anisotropy energy can be represented as the difference of the dipole-dipole interaction energies: $\Delta E_{dd} = E_{dd}\left(\overrightarrow{m_{\perp}}\right) - E_{dd}\left(\overrightarrow{m_{\parallel}}\right)$, in turn the expression for finding the dipole-dipole interaction energy is as follows:

$$E_{dd} = \frac{1}{c^2} \sum_{i \neq j} \left[\frac{\overrightarrow{m_i} \cdot \overrightarrow{m_j}}{\left|\overrightarrow{R_{ij}}\right|^3} - 3 \frac{\left(\overrightarrow{m_i} \cdot \overrightarrow{R_{ij}}\right)\left(\overrightarrow{m_j} \cdot \overrightarrow{R_{ij}}\right)}{\left|\overrightarrow{R_{ij}}\right|^5} \right]. \quad (5)$$

2. Results

The information in Tab. 1 presents the computed magnetic moment values of atoms within cobalt films ranging from 1 to 8 monolayers, accompanied by varying copper thicknesses from 3 to 9 monolayers in comparison with experimental data.

Table 1. Values of magnetic moments of Co atoms in the film

№, ат.	N_{Co}=1			N_{Co}=2			N_{Co}=3		
	$\mu_{tot}/at, \mu_B$								
	∥	⊥	Exp.	∥	⊥	Exp.	∥	⊥	Exp.
1	1.870	1.863	1.891 [4]	1.789	1.789	1.730 [5]	1.874	1.873	1.810 [6]
2				1.596	1.598		1.648	1.648	
3							1.654	1.654	

№, ат.	N_{Co}=4		N_{Co}=5		N_{Co}=6	
	μ_{tot}/at, μ_B					
	∥	⊥	∥	⊥	∥	⊥
1	1.841	1.841	1.852	1.852	1.846	1.846
2	1.659	1.661	1.656	1.657	1.657	1.658
3	1.642	1.644	1.694	1.696	1.670	1.670
4	1.600	1.603	1.642	1.644	1.669	1.669
5			1.627	1.630	1.647	1.647
6					1.617	1.616

It can be concluded that the different spin configurations have a weak effect on the values of magnetic moments.

Fig. 2, we show the dependence of the energies of magnetic anisotropy, spin-orbit interaction and shape anisotropy on the thickness of the considered material. These values were calculated in the VASP [7–10] program complex using the [11] technique. The number of monolayers of cobalt magnetic material varied from 1 to 8. The thickness of copper was constant and equal to 3 monolayers.

The graph shows the curves describing the behavior of the magnetic anisotropy energy. It was calculated as $(\Delta E_{SOC} + \Delta E_{dd})$ as the sum of the energies of spin-orbit and dipole-dipole interactions and (E_{MA}) as the difference of the total energies of the system at different directions of magnetic moments. We observe concurrence in the behavior of curves.

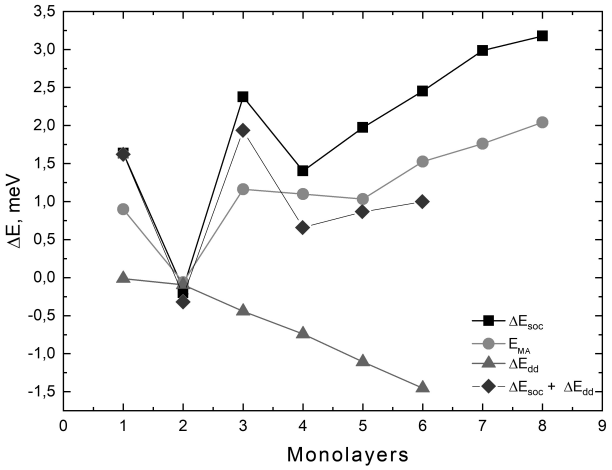

Fig. 2. Values of magnetic anisotropy, spin-orbit interaction and shape anisotropy energies as a function of the number of monolayers of magnetic cobalt material

The extended set of magnetic anisotropy, spin-orbit interaction and shape anisotropy energy values, taking into account the variable copper thickness (from 3 to 9 monolayers), is given in Tab. 2.

Table 2. Values of magnetic anisotropy, spin-orbit interaction and shape anisotropy energies as a function of the number of monolayers of copper substrate and cobalt magnetic material

N_{Co}	N_{Cu}	E_{MA}	ΔE_{SOC}, meV	E_{dd}, meV
	3	0,898	1,636	–0,01218
	5	0,944		
	7	0,899	1,560	–0,00195
1	9	0,930	1,641	–0,00139
	3	–0,062	–0,142	–0.095
	5	0,092	0,053	–0,080
	7	0,038	0,073	–0,077
2	9	–0,104	0,043	–0,076
	3	1,161	2,377	–0,442
	5	1,508	2,257	–0,422
	7	1,273	2,353	–0,415
3	9	1,152	2,311	–0,412

Weak magnetic anisotropy was found for the thickness of the magnetic material of cobalt 2 monolayers. The values of the spin-orbit interaction energy difference obtained by us are significantly larger than the energy difference of the dipole-dipole interaction, hence we can conclude that the main influence on the magnetic anisotropy energy is the contribution of magnetocrystalline anisotropy due to the spin-orbit interaction.

The ferromagnetic configuration of the system was calculated for facet (100) with a copper thickness varying from 3 to 9 monolayers and cobalt thickness from 1 to 8 monolayers.

Fig. 3 shows the calculated values of the anisotropy parameter compared with the values $\Delta = 1 - \dfrac{T_c(N)}{T_c(\infty)}$ obtained from the experimental critical temperatures $T_c(N)$ for Co/Cu(100) [12, 13] as a function of the number of cobalt monolayers. The data obtained are in good

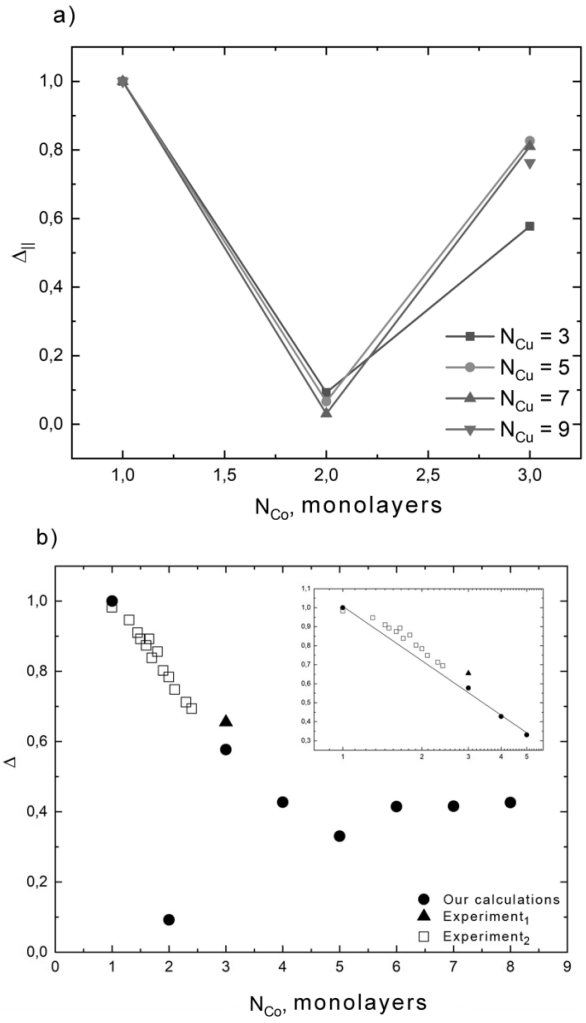

Fig. 3. (a) Calculated values of the magnetic anisotropy parameter as a function of the number of cobalt and copper monolayers (b) Calculated values of the anisotropy parameter as a function of the number of cobalt monolayers compared to values $\Delta = 1 - \frac{T_c(N)}{T_c(\infty)}$ obtained from experiments $T_c(N)$ for Co/Cu(100) (Experiment 1) [12] and (Experiment 2) [13]). The inset in the main plot shows the approximation of the values of the magnetic anisotropy parameter as a function of the number of cobalt monolayers on a logarithmic scale

agreement with experiment. The inset in the main plot shows the approximation of the values of the magnetic anisotropy parameter as a function of the number of cobalt monolayers (except $N_{Co} = 2$) on a logarithmic scale. The parameter $\lambda = 1.007$ calculated by us as the slope of the approximation line is close to the value of the scaling parameter $\lambda = 1.02$ given in the paper by [13] For the cobalt thickness of 2 monolayers, a "dropout" of the value of the magnetic anisotropy parameter associated with the change of the magnetic anisotropy energy both in sign and value is observed, which is summarized in Tab. 2. For the cobalt thickness of 2 monolayers, a "dropout" of the magnetic anisotropy parameter value associated with the change of the magnetic anisotropy energy both in sign and value is observed, which is shown in Tab. 2. Increasing the surface cell size (from 1 atom per layer to 4) and the thickness of the non-magnetic interlayer (from 3 to 9 monolayers) did not eliminate this feature. In contrast to the experiment, where

we considered partially filled layers, i.e., the film thickness varied from 1 to 2 monolayers with a step of 0.2, we considered a thickness multiple of a monolayer. The calculation of magnetic anisotropy requires the use of non-collinear calculations, the large resource intensity of which strongly depends on the number of atoms in the supercell. In the case of fully filled monolayers, it is sufficient to use 1 atom per layer, which was used in these calculations. In the case of partially filled monolayers, it is necessary to take 4 or 9 atoms in a layer, which increases the resource intensity of calculations by an order of magnitude.

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Исследование магнитной анизотропии пленок кобальта, разделенных слоем меди, в зависимости от толщины слоев

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Аннотация. Данная работа посвящена численному исследованию магнитных свойств системы Co/Cu/Co с использованием программного пакета VASP. Исследовано влияние вкладов магнитокристаллической анизотропии и анизотропии формы на энергию магнитной анизотропии. Получена зависимость энергий магнитной анизотропии, спин-орбитального взаимодействия и диполь-дипольного взаимодействия от толщины магнитного слоя кобальта.

Ключевые слова: магнитная анизотропия, сверхтонкие магнитные пленки, теория функционала спиновой плотности.