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First-principle calculations of the magnetic anisotropy of Fe and Co films separated by an interlayer of non-magnetic metals

© M.V. Mamonova, M.Yu. Makeev, D.S. Kalinin, A.A. Zenova

Dostoevsky Omsk State University,
Omsk, Russia

E-mail: mamonovamv@omsu.ru

Received July 8, 2021;
Revised July 8, 2021;
Accepted July 8, 2021

This paper presents the results of numerical calculations of the magnetic characteristics of Co and Fe monolayer films on Cu and Pt surfaces using the VASP software package. The values of the difference between the total energies of the antiferromagnetic and ferromagnetic configurations are calculated depending on the convergence parameters and the thickness of the nonmagnetic material. The values of the magnetic anisotropy and magnetic moment of atoms in the structures of Co/Cu/Co, Fe/Pt/Fe, Co/Pt/Co, Pt/Co/Cu/Co/Pt are determined depending on the orientation of the surface face. For the (110) and (111) faces, the phenomenon of reorientation in the Co/Cu/Co structure is confirmed, when the anisotropy of the cobalt films parallel to the surface plane is replaced by the perpendicular anisotropy due to the introduction of an ultrathin platinum film into the structure.

Keywords: Magnetic anisotropy, ultrathin magnetic films.

DOI: 10.21883/PSS.2022.13.52072.03s

1. Introduction

Recently, there has been a significant amount of interest in the properties of thin magnetic films. Such films are the key element of magnetic recording devices. In view of the rapid progress in magnetic recording technology, the calculation of magnetic properties in Co and Fe films has become a topical issue in solid-state physics.

The study of magnetic properties of multilayer structures [1] exhibiting giant magnetoresistance (GMR) is a pressing challenge, since these structures are used widely as read/write heads of hard disk drives, storage devices, and spintronic devices, the properties of which depend strongly on the magnitude of magnetic anisotropy. Multilayer structures with GMR effects consist of ferromagnetic layers separated by nonmagnetic layers. Owing to the oscillating RKKY interaction, the interlayer exchange constant varies with distance between the ferromagnetic layers. Adjusting the thickness of the nonmagnetic spacer material between two magnetic layers, one may alter the nature of interaction from ferromagnetic to antiferromagnetic. Therefore, it is crucial to estimate theoretically the thickness of the nonmagnetic layer that would make the antiferromagnetic configuration energetically favorable.

With the current density of magnetic storage approaching the superparamagnetic limit, it is believed that higher areal densities may be achieved by perpendicular recording, since the superparamagnetic limit is lower in magnetic media with perpendicular anisotropy [2]. While most systems feature in-plane magnetic anisotropy, multilayer Co/Pt structures with perpendicular anisotropy and, consequently, potential applications in extra-high density data storage have attracted much attention in recent years [3–6]. The perpendicular anisotropy in these systems is proportional to the interface area [7]. If the Co layer thickness is lower than the critical value (1 nm), the surface anisotropy exceeds the shape one, and a multilayer system becomes magnetized perpendicularly [8].

In order to calculate the magnetic anisotropy energy (MAE), we need to estimate the difference between the total energies of a magnetic material corresponding to different magnetization orientations. A stronger dependence on calculation parameters makes this task a computationally challenging one. Several studies into the magnetic moments and MAE in Co/Pt(111) and Fe/Pt(111) systems have already been published [9,10]. All these calculations utilized the fully relativistic screened Korringa–Kohn–Rostoker Green function method, the local density approximation, and the approximation of idealized geometry, which reproduces the three-dimensional structure of the substrate.

The present study is focused on examining the MAE of monolayer Fe and Co films on Cu and Pt within the SDFT formalism and calculating the self-consistent band structure in the VASP package. The differences between the results of MAE calculations carried out using different methods were analyzed in [11]. This study is distinct from the ones mentioned above in that we investigated not just ferromagnetic states, but also antiferromagnetic configurations with complete relaxation of the entire system formed by an adatom and the substrate. In addition, while calculations are often restricted to the (111) surface face, we examined the other orientations of surface faces

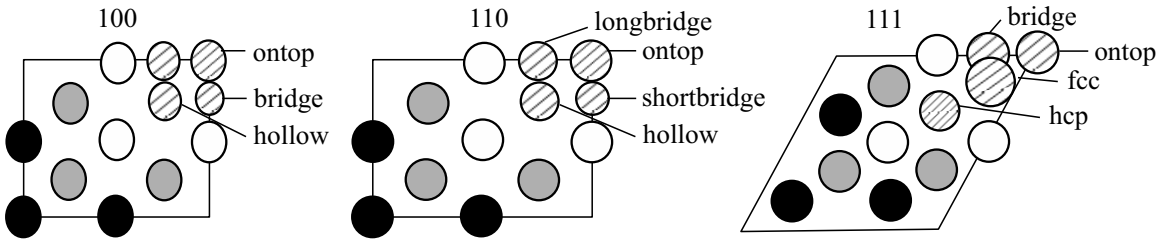

Figure 1. Configurations of adatom positions for different orientations of the surface face.

(specifically, (100), since it provides a square surface cell used in our Monte Carlo simulations) as well.

The experimental data [12] and the results of our Monte Carlo simulations [13,14] revealed that perpendicular anisotropy provides a beneficial magnetoresistance enhancement in a structure with ferromagnetic films containing $N < 11$ monolayers. Therefore, the aim of the present study was to examine the phenomenon of reorientation (observed experimentally in a Co/Cu/Co structure) in cobalt films with in-plane anisotropy, which changes to perpendicular anisotropy after an ultrathin platinum film is deposited on top of the structure, by first-principle calculations.

2. Model and methods

The spin-density functional theory is the basis for first-principle calculations of the electronic and crystal structure of magnetic materials. Multilayer structures were simulated in VASP [15] using the PAW method with the (PBE) version of the generalized gradient approximation (CGA). Collinear (with the magnetic moment set by a scalar) and noncollinear (with the magnetic moment set by a vector) magnetization configurations were applied. A Monkhorst–Pack k-point mesh was used in integration over the first Brillouin zone. The plane-wave basis cutoff energy was set to $E_{\text{cut}} = 500$ eV at a vacuum layer thickness of 5 Å. The size of the k-point mesh was varied from $5 \times 5 \times 1$ to $55 \times 55 \times 1$.

Table 1. Total energy E (eV) for Fe/Pt/Fe and Co/Pt/Co

Face	Adatom position	Fe/Pt	Co/Pt
100	ontop	−42.7	−39.60
	hollow	**−45.1**	**−42.34**
	bridge	−44.0	−41.23
110	ontop	−41.3	−37.20
	hollow	**−45.3**	**−42.71**
	longbridge	−43.6	−40.56
	shortbridge	−42.1	−39.24
111	ontop	−44.2	−41.21
	hcp	**−45.3**	−42.00
	fcc	−44.8	**−42.61**
	bridge	−45.3	−42.60

A film atom may be adsorbed onto the substrate in different positions, which are presented in Fig. 1. Therefore, calculations of the total energy of the supercell as a function of the surface face and the adatom position were performed for monolayer Fe and Co films on a Pt substrate with a thickness of 5 monolayers. The obtained results are presented in Table 1.

It may be concluded that the most energetically favorable position of both Fe and Co atoms on the Pt substrate is the interstitial one (hollow for the 100 and 110 faces and hcp or fcc for 111). In subsequent studies, the system was a nonmagnetic metal plate with a low-Miller-index surface face and ferromagnetic films adsorbed interstitially at both sides to preserve inversion symmetry.

A periodic supercell with a lattice constant corresponding to the substrate obtained in calculations (with the optimization of lattice parameters taken into account) was used to simulate the multilayer structure. The calculated equilibrium lattice parameters $a = 3.6367(5)$ Å for Cu and $a = 3.87125(3)$ Å for Pt are close to the corresponding experimental values ($a = 3.6153$ Å for Cu [16] and $a = 3.9158$ Åfor Pt [17]).

2.1. Examination of Favorability of Different Spin Configurations

Calculations for a monolayer ferromagnetic film on the Pt(100) surface in relation to the convergence parameters and the nonmagnetic interlayer thickness were carried out first. Complete relaxation of all layers of the supercell was performed.

The total energy for ferromagnetic (FM) and antiferromagnetic (AFM) spin configurations was calculated (Fig. 2). Let us introduce difference $\Delta E = E_{\text{afm}} - E_{\text{fm}}$ between the total energies of the system with the magnetic moments of atoms in films on two sides of the plate being directed oppositely (antiferromagnetic configuration) and codirectional (ferromagnetic configuration). At $\Delta E < 0$, the AFM orientation is more energetically favorable. At $\Delta E > 0$, the energetically favorable orientation is the FM one.

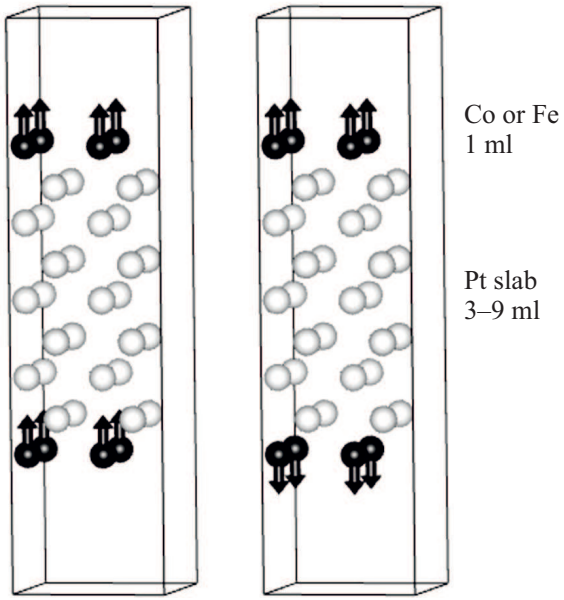

Figure 2. Crystal structure of the supercell and orientation of magnetic moments of atoms in the film.

The examination of convergence with respect to the number of k-points (mesh sampling points in integration over the first Brillouin zone) revealed that the convergence for ΔE (Fig. 4) is far worse than that for the total energy (Fig. 3). Thus, we need to use large numbers of k-points (mesh sizes on the order of $50 \times 50 \times 1$), while a mesh size of approximately $15 \times 15 \times 1$ is generally sufficient for calculations of the adsorption energy and magnetic moments. If the number of k-points is not sufficient, even the sign of ΔE may change (see Fig. 6, a).

However, it should be noted that such a significant increase in the number of k-points translates into sharply increased requirements for computer resources in terms of computation time and, most importantly, memory (Fig. 5).

The results of calculation of ΔE for Fe and Co films adsorbed onto both sides of the Pt(100) in relation to the plate thickness are presented in Fig. 6.

The calculations demonstrated that the FM orientation remains more energetically favorable for a Co film with a thickness of 1 and 2 monolayers at all the studied values of the Pt plate thickness and gives way to the AFM orientation only in the case of a three-layer Co film at Pt thickness in excess of 5 monolayers.

The antiferromagnetic orientation is favorable for a monolayer Fe film at all the studied Pt thickness values. However, the value of ΔE for Fe (approximately 1 meV) is much lower than the corresponding value for Co.

Thus, it may be concluded that the emergence of antiferromagnetic interaction between two magnetic layers is affected by the thickness of both the nonmagnetic material and magnetic layers.

2.2. Calculations of Magnetic Anisotropy

Next, let us consider multilayer structures with the thickness of each layer equal to 3 ml (Fig. 7) in relation to the magnetization direction and the orientation of the surface face.

Magnetic anisotropy energy $E_{\mathrm{MA}} = E_{\perp} - E_{\parallel}$ is the difference between the total energies of systems with their magnetization being perpendicular and parallel to the surface plane. At $E_{\mathrm{MA}} < 0$, the orientation of magnetic moments perpendicular to the surface is more energetically favorable. This corresponds to easy-axis anisotropy. At $E_{\mathrm{MA}} > 0$, the orientation of magnetic moments parallel to the surface is more energetically favorable. This corresponds to easy-plane anisotropy.

The results of calculation of the difference in total energy for different spin configurations of structures based on cobalt

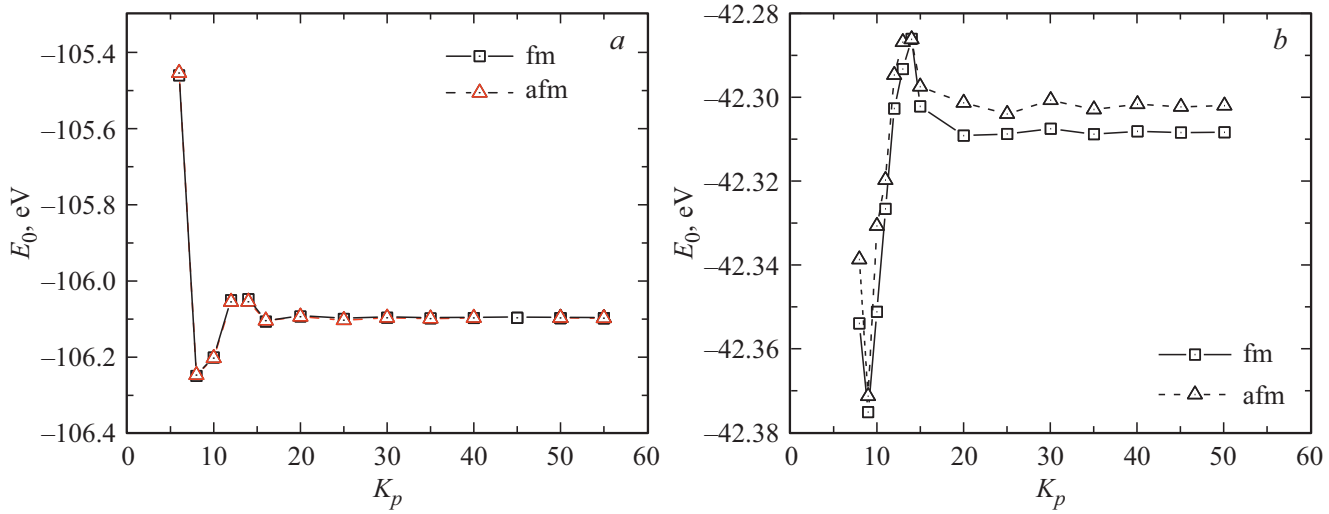

Figure 3. Convergence of the total energy with respect to the number of k-points (K_p) for Fe/Pt/Fe (a) and Co/Pt/Co (b).

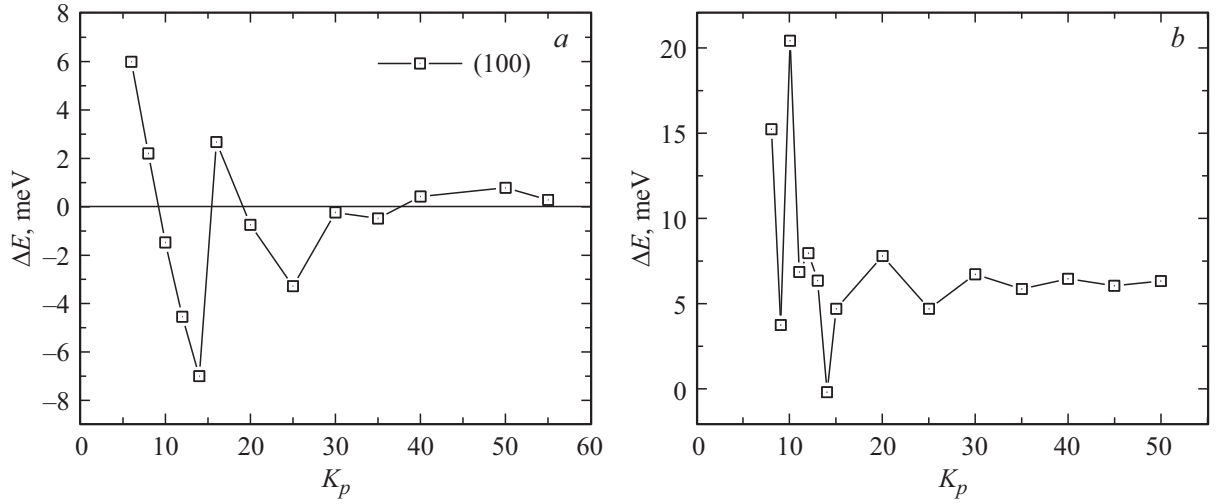

Figure 4. Convergence of the energy difference between the AFM and FM configurations with respect to the number of k-points (K_p) for Fe/Pt/Fe(a) and Co/Pt/Co (b).

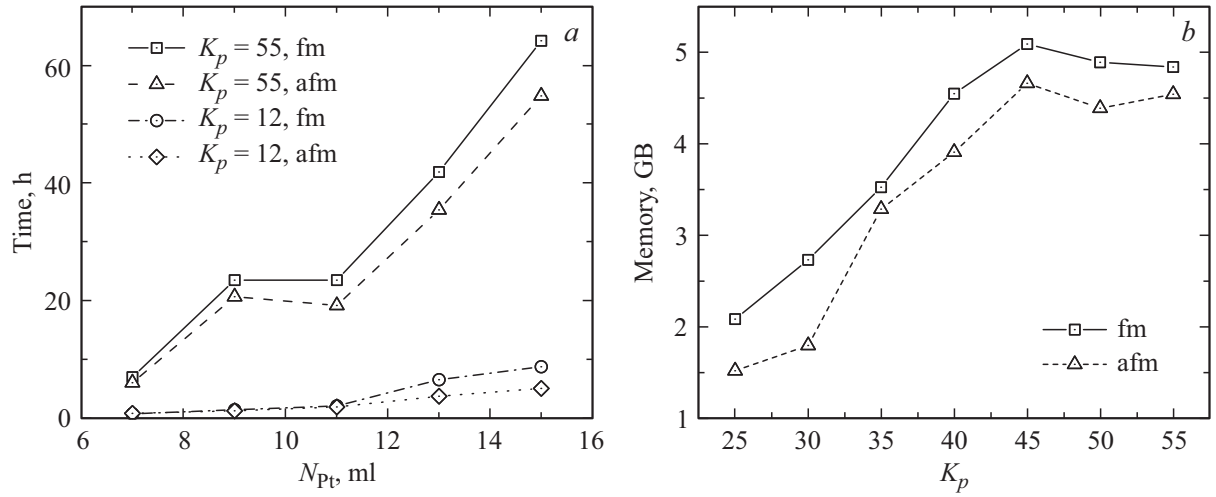

Figure 5. Dependences (a)of the computation time on the Pt plate thickness for meshes $12 \times 12 \times 1$ and $55 \times 55 \times 1$ in size and (b)the required memory amount per core on the number of k-points (K_p) for the AFM and FM configurations of Fe/Pt/Fe.

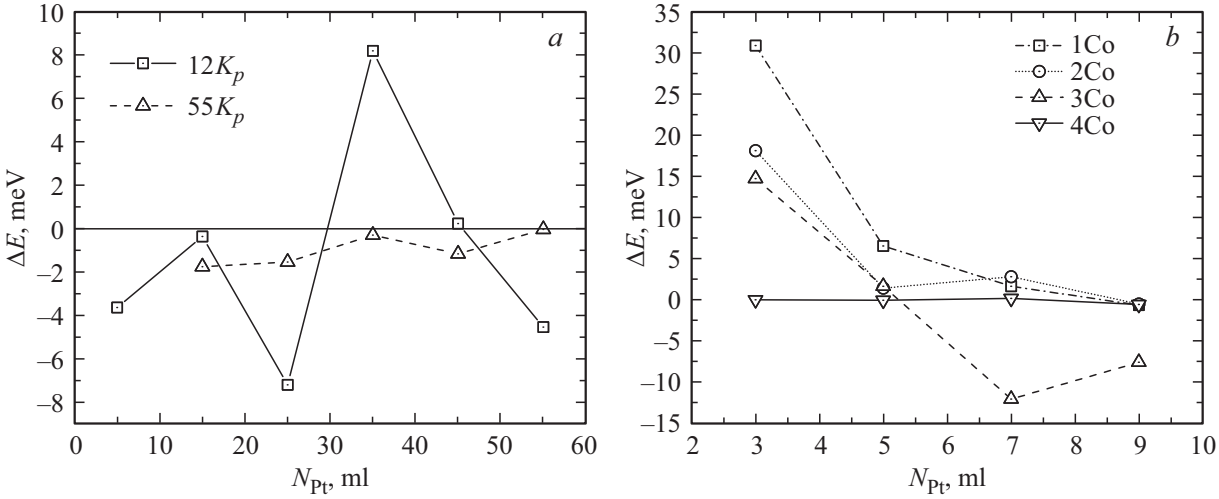

Figure 6. Dependences of the energy difference between the AFM and FM configurations on the Pt plate thickness for Fe/Pt/Fe (a) and Co/Pt/Co (b) at different mesh sizes.

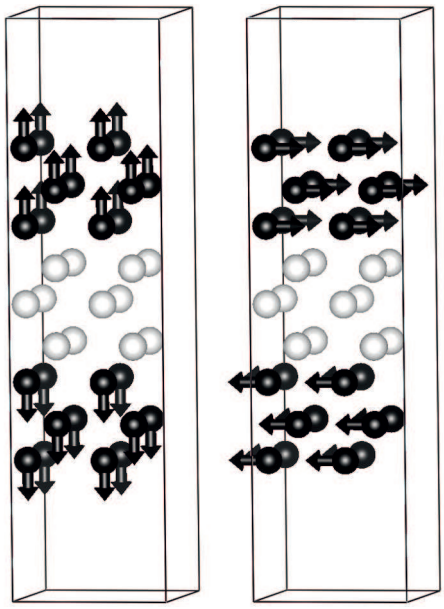

Figure 7. Crystal structure of the supercell and orientation of magnetic moments of atoms in the film.

films with a nonmagnetic platinum or copper interlayer and with a platinum film deposited on top of the Co/Cu/Co structure are presented in Tables 2 and 3.

The results of calculation of energy difference ΔE between the AFM and FM configurations of cobalt films with a copper interlayer revealed that the FM configuration is more favorable for the (100) face, while the AFM configuration is favorable for the other faces. The deposition of an additional Pt layer on top of Co/Cu/Co alters the sign of ΔE only for the (111) face. The FM configuration remains favorable for cobalt films with a platinum interlayer in almost all the studied cases.

It is known from experiment [12] that the Co/Cu structure is characterized by weak easy-plane anisotropy with in-plane magnetization. However, if ultrathin platinum films are deposited onto cobalt films, the obtained Pt/Co/Cu/Co/Pt structure is instead characterized by easy-axis anisotropy with magnetization perpendicular to the film plane. Our calculations corroborate these findings. The Co/Cu/Co structure has $E_{MA} = E_{\perp} - E_{\parallel} > 0$, which corresponds to easy-plane anisotropy. The only exceptions are very small values of $E_{MA} = -0.05$ eV for the energetically unfavorable FM configurations of the (110) and (111) faces. As was noted in [12], additional measurements performed by Kohlhepp et al. (1992) and den Broeder et al. (1991) have confirmed that the Co/Cu(111) system does indeed exhibit weak anisotropy perpendicular to the interface on the order of 0.1 mJ/m^2.

At the same time, easy-axis anisotropy with magnetization perpendicular to the film plane emerges in the Pt/Co/Cu/Co/Pt structure for the FM configuration of the (110) face and in the Co/Pt/Co structure for the AFM configuration of the (111) face. This agrees with the experimental data [12], since perpendicular magnetic anisotropy was observed in these structures specifically for the (111) face.

The results of MAE calculations revealed that in the case of the (100) surface face orientation, all the examined structures based on cobalt films with a nonmagnetic platinum or copper interlayer and with a platinum film deposited on top of the Co/Cu/Co structure are characterized by easy-plane anisotropy with in-plane magnetization.

The results of calculation of the magnetic moment of Co atoms for the examined systems are presented in Table 4. The magnetic moment of Co is the greatest in Co/Pt/Co and the smallest in the Co/Cu/Co system. The average magnetic moment of Co atoms (Table 4) is the greatest in the structure with a platinum interlayer and depends weakly on the spin configuration (the difference is approximately $0.01\,\mu_B$).

Next, let us consider structures based on an iron film in relation to the orientation of the surface face. The results of calculation of the magnetic anisotropy energy and magnetic

Table 2. Results of calculation of energy difference ΔE between the AFM and FM configurations for different orientations of the surface face and magnetization directions

Face	Ordering type	ΔE, meV		
		Co/Pt/Co	Co/Cu/Co	Pt/Co/Cu/Co/Pt
100	$\parallel$	12.344	9.466	16.000
	$\perp$	12.889	6.631	17.034
110	$\parallel$	5.592	−31.784	−30.755
	$\perp$	8.426	−31.585	−28.443
111	$\parallel$	4.965	−7.160	3.448
	$\perp$	−1.406	−6.854	3.077

Table 3. Results of calculation of MAE $E_{MA} = E_{\perp} - E_{\parallel}$ for different orientations of the surface face

Face	Spin configuration	E_{MA}, meV		
		Co/Pt/Co	Co/Cu/Co	Pt/Co/Cu/Co/Pt
100	FM	0.965	3.204	1.961
	AFM	1.510	0.369	2.995
110	FM	0.993	−0.050	−2.205
	AFM	3.827	0.149	0.107
111	FM	0.463	−0.044	−0.034
	AFM	−5.908	0.262	−0.405

Table 4. Results of calculation of average magnetic moment μ, μ_B of Co atoms and magnetic moment μ_1, μ_B of the Co atom closest to the nonmagnetic interlayer

Face	Ordering type		Co/Pt/Co		Co/Cu/Co		Pt/Co/Cu/Co/Pt	
			μ, μ_B	μ_1, μ_B	μ, μ_B	μ_1, μ_B	μ, μ_B	μ_1, μ_B
100	FM	$\parallel$	1.765	1.851	1.724	1.885	1.751	1.836
		$\perp$	1.764	1.850	1.721	1.871	1.753	1.835
	AFM	$\parallel$	1.766	1.847	1.721	1.870	1.752	1.834
		$\perp$	1.765	1.847	1.722	1.872	1.751	1.831
110	FM	$\parallel$	1.854	1.889	1.732	1.871	1.833	1.884
		$\perp$	1.850	1.893	1.732	1.867	1.834	1.892
	AFM	$\parallel$	1.848	1.896	1.721	1.854	1.835	1.893
		$\perp$	1.847	1.894	1.721	1.855	1.835	1.893
111	FM	$\parallel$	1.814	1.853	1.701	1.773	1.805	1.858
		$\perp$	1.814	1.854	1.701	1.775	1.805	1.856
	AFM	$\parallel$	1.812	1.850	1.702	1.780	1.805	1.856
		$\perp$	1.812	1.852	1.701	1.774	1.806	1.857

Table 5. Results of calculation of μ, μ_B for a monolayer Fe film and a Pt plate thickness of 9 ml in comparison with the results of calculations within the KKR formalism for a Pt substrate thickness of 37 ml [19] and a semi-infinite Pt surface [10]

Ordering type	(111)	(110)	(100)
$\parallel$	2.98 3.018 [10]	3.15	3.06
$\perp$	2.97 2.92 [19] 3.016 [10]	3.15	3.05

moments for monolayer iron films separated by a platinum interlayer are presented in Fig. 8 and Table 5. It can be seen that perpendicular anisotropy emerges in monolayer iron films with a platinum interlayer only for the (100) face (at all the examined Pt thickness values) and the (110) face (at a Pt plate thickness of 5 monolayers). Meanwhile, easy-plane anisotropy with $E_{MA} = E_\perp - E_\parallel \approx 0.5{-}1.0$ meV is more energetically favorable for the (111) face at all thicknesses of the nonmagnetic interlayer.

The results of our calculations for the (111) face agree with calculated data presented in other studies. The adsorption of iron clusters of various geometries (down to a monolayer) onto the Pt (111) surface face was investigated in [19]. Calculations were performed within the Korringa–Kohn–Rostoker (KKR) formalism [18] for a Pt substrate thickness of 37 ml. No effects of structure relaxation were included, and the k-mesh size was $100 \times 100 \times 1$. The easy-axis MAE was prevalent for all the studied clusters of the Fe/Pt(111) system. However, easy-plane anisotropy with $E_{MA} = E_\perp - E_\parallel = 0.26$ meV was found to be prevalent in calculations for a monolayer. The calculations for a single Fe monolayer on Pt(111) carried out in [10] revealed planar

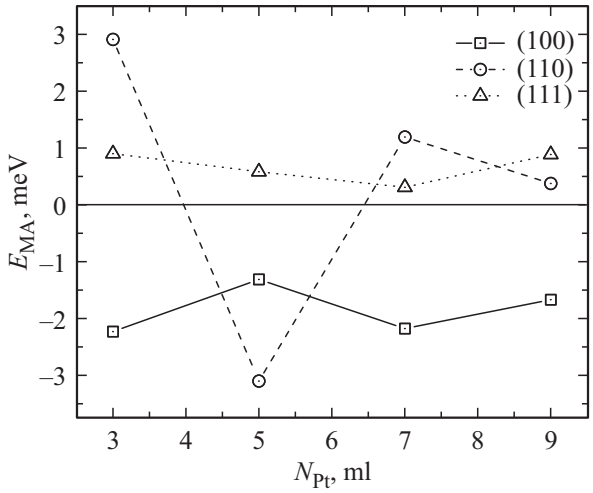

Figure 8. Magnetic anisotropy value for the 1Fe/Pt/1Fe system as a function of the platinum interlayer thickness for different orientations of the surface face.

Table 6. Results of calculation of magnetic anisotropy E_{MA}, meV and magnetic moments μ, μ_B of Fe atoms and the near-surface Pt layer for the 3Fe/3Pt/3Fe system with different orientations of the surface face

Face		E_{MA}, meV	μ_{Pt}	μ_{Fe1}	μ_{Fe2}	μ_{Fe3}
100	$\perp$	−1.57	0.293	2.752	2.399	2.906
	$\parallel$		0.283	2.748	2.402	2.893
110	$\perp$	−1.10	0.358	2.842	2.800	2.848
	$\parallel$		0.357	2.842	2.801	2.848
111	$\perp$	−1.45	0.273	2.833	2.588	2.852
	$\parallel$		0.266	2.835	2.592	2.859

magnetic anisotropy $E_{MA} = 0.71$ meV, while a single Fe adatom on Pt(111) was strongly perpendicularly oriented.

The results of calculation of the magnetic anisotropy energy and magnetic moments for iron films separated by a platinum interlayer with the thickness of each material being equal to 3 monoatomic layers are presented in Table 6.

It was found that perpendicular anisotropy emerges for all orientations of the surface face of iron films with a thickness of 3 monoatomic layers, but only for the (100) face in the case of a monoatomic film.

3. Conclusion

We note in conclusion that first-principle calculations of the magnetic anisotropy of Co and Fe films separated by a Cu or Pt plate were carried out in the present study. The dependence of anisotropy on the convergence parameters and the plate thickness was investigated. The examination of convergence with respect to the number of k-points revealed that the convergence for ΔE is far worse than that for the total energy. Thus, we need to use large numbers of k-points (meshes approximately $50 \times 50 \times 1$ in size).

The ferromagnetic orientation remains more energetically favorable for a Co film with a thickness of 1 and 2 monolayers at all the studied values of the Pt plate thickness and gives way to the antiferromagnetic orientation only in the case of a three-layer Co film at Pt thickness upwards of 7 monolayers. The antiferromagnetic orientation is favorable for a monolayer Fe film at all the studied Pt thickness values.

The values of MAE and the magnetic moments of atoms in Fe/Pt/Fe, Co/Cu/Co, Co/Pt/Co, and Pt/Co/Cu/Co/Pt structures with each metal having a thickness of 3 monolayers were determined for different orientations of the surface face. The Co/Cu/Co structure is characterized by easy-plane anisotropy; very weak perpendicular anisotropy was found only for the energetically unfavorable FM configurations of the (110) and (111) faces.

However, if ultrathin platinum films are deposited onto cobalt films (specifically, the (111) face and the FM configuration of the (110) face), the obtained Pt/Co/Cu/Co/Pt structure is instead characterized by easy-axis anisotropy. In calculations for Co/Pt/Co, perpendicular anisotropy turned out to be more energetically favorable for the AFM configuration of the (111) face.

In the case of the (100) surface face orientation, all the examined structures based on cobalt films with a nonmagnetic platinum or copper interlayer and with a platinum film deposited on top of the Co/Cu/Co structure are characterized by easy-plane anisotropy.

Perpendicular anisotropy emerges for all orientations of the surface face of iron films with a thickness of 3 monoatomic layers, but only for the (100) face in the case of a monoatomic film.

Our conclusions agree with the experimental data reviewed in [12] and the results of calculations carried out in [19,10]. The obtained results may find application in numerical Monte Carlo simulations of the nonequilibrium behavior of multilayer magnetic superstructures [20].

Funding

This study was supported financially by the Russian Foundation for Basic Research (project No. 20-32-70189), the Ministry of Science and Higher Education of the Russian Federation (agreement 0741-2020-0002), and grant MD-2229.2020.2 from the President of the Russian Federation. Computational resources of the Common Use Center of the Far Eastern Branch of the Russian Academy of Sciences (Khabarovsk) were used.

Conflict of interest

The authors declare that they have no conflict of interest.

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