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First-principles investigation of magnetism of U films and $U(001)_1/Fe(110)_3$ multilayers

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Abstract

The magnetism of surfaces and interfaces can differ strongly from the magnetism of corresponding bulk materials. In the case of actinide systems the study of the surfaces and interfaces is still at the very beginning. In this work, we investigated the electronic and magnetic properties of U films and $U(001)_1/Fe(110)_3$ multilayers within the framework of the density functional theory. We report both scalar-relativistic and fully relativistic calculations. The exchange correlation potential was treated in the generalized gradient approximation (GGA). In agreement with previous calculation by Stojić *et al* (2003 *Phys. Rev.* B **68** 094407) we obtained the surface layer of the U films to be magnetic for the bulk lattice parameter. The dependence of the magnetic properties of the U films on the lattice parameter was studied. It is shown that decreasing distances between U atoms lead to decreasing magnetic moment and finally to the nonmagnetic ground state. The variation of the magnetic moment as a function of the lattice parameter is discontinuous. Using the frozen-magnon approach we evaluated the parameters of the inter-atomic exchange interactions and estimated the Curie temperature. The calculation for $U(001)_1/Fe(110)_3$ multilayers showed that the U layer is magnetic with the direction of the U moments opposite to the Fe moments. The importance of the U–Fe hybridization is revealed. Both the intra-layer (U–U, Fe–Fe) and inter-layer (U–Fe) exchange interactions were evaluated. The temperature dependence of the layer magnetizations was studied within the random-phase approximation for the Heisenberg Hamiltonian for classical spins.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The magnetism of surfaces and interfaces of transition metals attracts considerable experimental and theoretical attention. The reduced symmetry, the lower coordination number and localized surface and interface states open the possibility of the formation of new and exotic magnetic phenomena. An interesting result in the physics of low-dimensional systems

is the discovery of the magnetic state of the surfaces for materials that are nonmagnetic in the bulk [1]. For example, the magnetic states have been predicted for the 4d and 5d metals. In the 4d series, monolayer magnetism has been predicted for Tc, Ru, and Rh [2–7]. Within the 5d series, Os and Ir [2, 3] were found to be magnetic. Magnetic behaviour has also been predicted for isolated clusters [8–12], for small clusters deposited on silver [13], and in epitaxial ultrathin layers deposited on Rh(001) and Pd(001) surfaces [14, 15].

Metallic vanadium is known to be non-magnetic. However, the calculations indicate that an expansion of the lattice constant [16] and changes in the coordination number at the surface [17] may induce a magnetic state. As a rule, one expects an increased tendency toward magnetism near metal surfaces since the narrowing of the energy bands yields a Stoner enhancement of the spin susceptibility that leads to the instability of the nonmagnetic state.

Magnetism was theoretically predicted for a monolayer of transition metals on noble-metal substrates such as Ti, V, Ru, and Rh on Ag or Au [18]. Experimentally, the situation is less clear. In the other hand, the existence of two-dimensional magnetic order at the Rh(100) surface has been a controversial issue. Surface magnetism has been detected in the Rh(100) system that is nonmagnetic in the bulk [19, 20]. Another suggestion is that the magnetic state of the Rh(100) surface could be super-paramagnetic [21]. The discovery of the surface magnetism of a nonmagnetic material can be technologically interesting and it can find applications in the magnetic storage industry.

The physics of actinide systems with two-dimensional translational symmetry forms a challenging and practically unexplored field of research. The actinides and actinide compounds exhibit a broad spectrum of magnetic behaviour, such as Pauli paramagnetism, localized- and itinerant-electron magnetism and the magnetism of heavy-fermion systems [22, 23]. It can be expected that in many actinide systems the magnetic properties of the bulk will be different from the properties of the corresponding materials with two-dimensional symmetry. An interesting candidate for the investigation of the magnetism of low-dimensional materials is the 5f element uranium (U). A uranium atom has three 5f electrons. The 5f bands of actinide metals are in general narrower than the 3d bands of the 3d transition metals. Combined with the band-narrowing effect of the surface [24], this property of the 5f bands can result in the formation of a surface magnetic state. Stojić *et al* [25] performed a first-principles study of U films and found the ground state of the surface layer to be ferromagnetic despite the paramagnetic ground state of the bulk uranium.

Magnetic multilayers have recently attracted a great deal of interest, based not only on their potential technical applications, but also on understanding the fundamental mechanisms of their magnetic properties. Interest in rare-earth multilayers arises because of their earlier interest in U-based multilayers [26, 29] where there is a strong interaction between the 5f electrons of U and the 3d electrons of transition metals, giving rise to interesting properties. Recently, pioneer experimental studies of U/Fe multilayers [26, 29] have been reported. In the form of compounds, the U–Fe systems have been studied intensively, both experimentally and theoretically [30–34]. Magnetism in uranium compounds is defined by the large orbital moment of the 5f electrons, with attendant large anisotropy, and strong hybridization that occurs between the 5f electrons and the valence band states of neighbouring atoms. Accordingly, the study of uranium-based multilayers is a potentially important extension of the study of multilayers. But, the difficulty one faces in the fabrication of the U/Fe multilayers is related to the strong mismatch in the lattice parameters of Fe and U: the surface lattice parameter of the Fe(110) surface differs from the U(001) lattice parameter by 30%. Thomas *et al* [26, 27] produced U/Fe(110) multilayers by dc magnetron sputtering. They have investigated the magnetic properties of the system by polarized neutron reflectivity (PNR). In particular, the question about the magnetic state of the U atoms in the vicinity of the iron layers was addressed.

The PNR results show that the magnetic moment of the iron layers is reduced compared to the moment of pure bcc iron, and they set an upper limit on any moment on the U layers. Beesley *et al* [28, 29] determined the Curie temperatures for U/Fe multilayers from ac susceptibility measurements and found the T_C values to be less than the value of 1045 K for bulk Fe. With the technique employed, they have been unable to observe any magnetism of the U layers. However, an earlier resonant x-ray scattering (RXS) study [27] on U/Fe multilayers has shown that the 5f states are polarized.

The aim of the present work is the theoretical study of the magnetic and electronic properties of the slabs with several U layers and $U(001)_1/Fe(110)_3$ multilayers. The calculations were performed within the framework of the density functional theory (DFT) using the augmented spherical waves (ASW) method [35].

We investigated the effect of the lattice contraction on the magnetic properties of the U surface. For the first time, we investigated the exchange coupling between the atomic magnetic moments at the U surface. We employed the frozen-magnon approach to calculate the interatomic exchange parameters. Our results show that the intra-layer exchange coupling is short range. Despite recent experiments reported on the magnetic properties of U/Fe multilayers, there is no theoretical study devoted to the calculation of exchange parameters. We used the calculated exchange parameters to estimate the Curie temperature in the RPA approximation. The calculations of the temperature dependence of magnetization are presented.

The paper is organized as follows. In section 2 we present the calculational scheme. Section 3 contains the results of the calculations and discussion. Section 4 is devoted to concluding remarks.

2. Calculational scheme

The calculations reported in the paper have been carried out with the ASW method [35] in the scalar relativistic and fully relativistic versions (with and without spin orbit coupling (SOC), respectively). For the exchange–correlation potential, we employed the GGA approximation. The calculations have been carried out using the face-centred-orthorhombic structure of α-U (figure 1(a)). The unit cell of this structure contains two atoms. We used the following lattice parameters: $a = 2.836$ Å, $b = 5.866$ Å, $c = 4.935$ Å, and $y = 0.1017$ [37]. The structure belongs to the non-isomorphic space group $Cmcm$. The calculations were performed for films containing an odd number of atomic layers in the range from 1 to 7. To simulate vacuum, five layers of empty spheres have been used. For the calculations of one monolayer (ML) we used 200 **k**-points in the irreducible part of the two-dimensional Brillouin zone. For the films with several monolayer the number of **k**-points varied from 250 for the 3 ML film to 130 for the 7 ML film.

For $U(001)_1/Fe(110)_3$ multilayers, we considered the system consisting of periodically repeated 1 ML of U(001) and 3 ML of Fe(110). The comparison of the in-plane lattice parameters corresponding to the bulk lattices of Fe and U shows that one of the lattice parameters is very similar in both cases (mismatch of 0.6%) while the second parameter differs strongly (mismatch of more than 30%). This strong mismatch is a serious problem for growing Fe–U multilayers with well characterized interfaces [26, 29]. The calculations reported here were performed for the simplified lattice model depicted in figure 1(b). As the lattice constant of the multilayers, adopting Fe(110) lattice type, we chose the average between Fe and U lattice constants in the plane and in the perpendicular direction.

To calculate the interatomic exchange interactions we used the frozen-magnon technique [38] and mapped the results of the calculation of the total energy of the helical

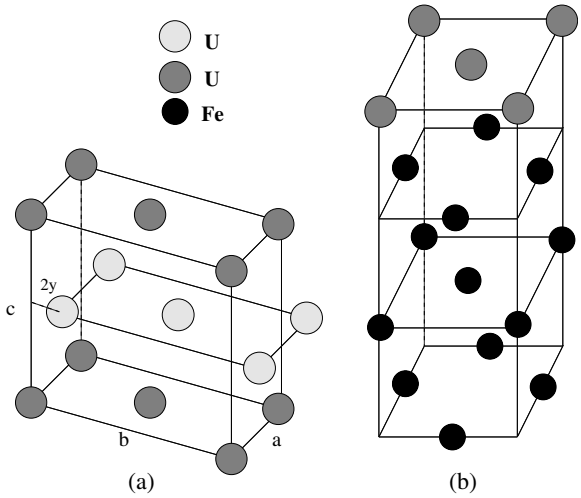

Figure 1. (a) Schematic representation of the α-uranium structure. (b) Supercell geometry considered to simulate the $U(001)_1/Fe(110)_3$ multilayers.

magnetic configurations

$$\mathbf{s}_n = (\cos(\mathbf{q}\mathbf{R}_n)\sin\theta, \sin(\mathbf{q}\mathbf{R}_n)\sin\theta, \cos\theta) \tag{1}$$

onto a classical Heisenberg Hamiltonian

$$H_{\text{eff}} = -\sum_{i\neq j} J_{ij}\mathbf{s}_i\mathbf{s}_j \tag{2}$$

where J_{ij} is the exchange interaction between two U sites and $\mathbf{s}_i$ is the unit vector pointing in the direction of the magnetic moment at site i. The $\mathbf{R}_n$ are lattice vectors, $\mathbf{q}$ is the wavevector of the helix, θ the polar angle giving the deviation of the moments from the z axis. Within the Heisenberg model (2), the energy of frozen-magnon configurations can be represented in the form

$$E(\theta, \mathbf{q}) = E_0(\theta) - \sin^2\theta J(\mathbf{q}) \tag{3}$$

where E_0 does not depend on $\mathbf{q}$ and $J(\mathbf{q})$ is the Fourier transform of the parameters of exchange interaction between pairs of U atoms:

$$J(\mathbf{q}) = \sum_{\mathbf{R}} J_{0\mathbf{R}}\ \exp(\mathrm{i}\mathbf{q}\cdot\mathbf{R}). \tag{4}$$

Calculating $E(\theta, \mathbf{q})$ for a regular $\mathbf{q}$-mesh in the Brillouin zone of the crystal and performing inverse Fourier transformation one gets exchange parameters $J_{0\mathbf{R}}$ between pairs of U atoms. The Curie temperature was estimated in the random phase approximation (RPA)

$$\frac{1}{k_{\text{B}}T_{\text{C}}^{\text{RPA}}} = \frac{6\mu_{\text{B}}}{M}\frac{1}{N}\sum_{\mathbf{q}}\frac{1}{\omega(\mathbf{q})+\Delta} \tag{5}$$

where $\omega(\mathbf{q}) = \frac{4}{M}[J(0) - J(\mathbf{q})]$ is the energy of spin-wave excitations and Δ is the magnetic anisotropy energy. We used the RPA approach to study the temperature dependence of the magnetization in the temperature interval from 0 K to T_{C}. The RPA technique for a multi-sublattice system is presented in [36].

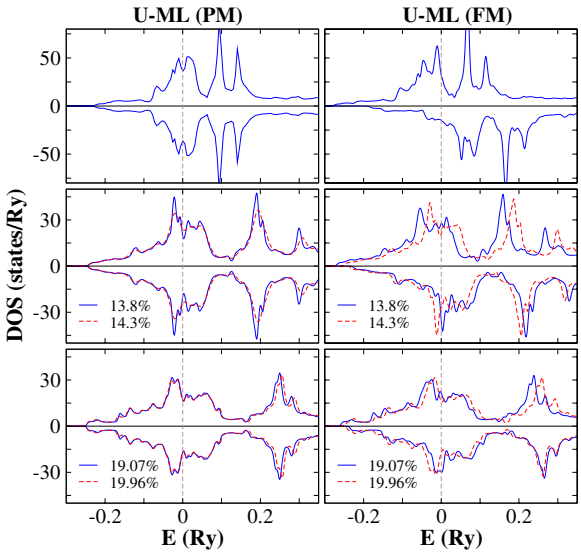

Figure 2. Densities of states of free-standing U monolayer. The left-hand panels present nonmagnetic densities of states for various lattice constants. The upper panel shows the DOS for the bulk lattice constant. The lower two panels present the DOS for contracted lattices. The values of the volume contraction are given in the figures and correspond to the critical points in the volume dependence of the magnetic moment (see figure 4 and the discussion in the text). The right-hand panels present the ferromagnetic DOS for the same lattice parameters. The Fermi level is given by the vertical dashed line.

3. Results and discussions

3.1. Magnetism of uranium films

3.1.1. Density of states and magnetic moments of U(001) surface. We begin with the discussion of the calculational results for the 1 ML film. In figure 2, we present the density of states (DOS) for different lattice spacings. The contraction of the lattice constant up to 19.96% with respect to the experimental value is considered. The calculations were performed for both nonmagnetic and ferromagnetic states. The left panels in figure 2 contain the DOS of the nonmagnetic state. The decrease of the lattice constant leads to the broadening of the energy bands that results in decreasing of DOS at the Fermi level, $N(E_F)$. According to the Stoner criterion, the higher the density of states at the Fermi level the stronger is the instability of the nonmagnetic state with respect to formation of the ferromagnetic state. In figure 3(a) the dependence of $N(E_F)$ on the lattice parameter is presented. As expected, the value of the DOS decreases monotonically with the contraction of the lattice. The dependence is close to linear.

The right-hand panel of figure 2 contains the DOS obtained in the spin-polarized calculations. In contrast to the bulk case the magnetic moment of the 1 ML system did not disappear within the iterational process and the calculations resulted in a ferromagnetic state. The values of the magnetic moments for the bulk lattice constant are collected in table 1. The results are presented for both scalar-relativistic and fully relativistic calculations.

Because of the lower coordination number for the surface atoms the width of the 5f bands in low-dimensional U systems is considerably narrower than in the bulk. The narrowing of the bands leads to an increased DOS at the Fermi level. According to the Stoner criterion for the ferromagnetic instability $N(E_F)I > 1$, the increased DOS at the Fermi level enhances

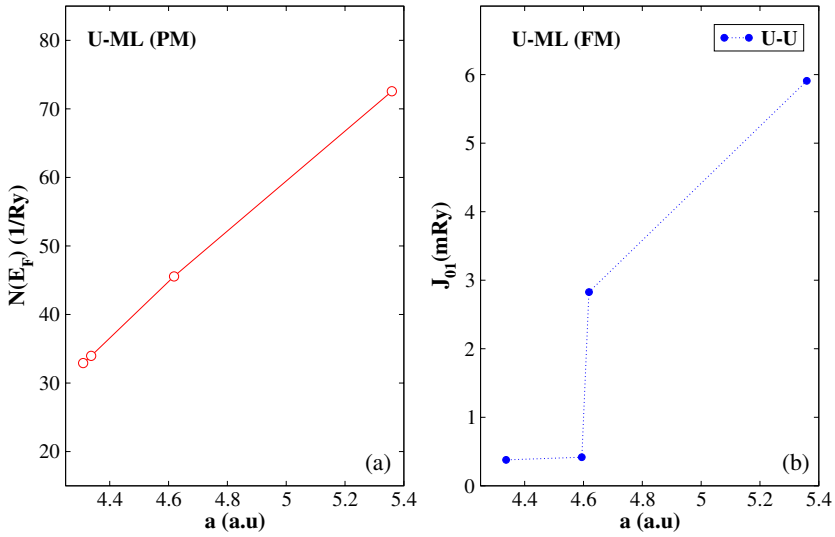

Figure 3. (a) The density of states at the Fermi level at critical points of the lattice contraction for 1 ML. (b) The dependence of the parameter of the exchange interaction between nearest U neighbours on the lattice contraction.

Table 1. Calculated spin (spin and orbital) magnetic moments for the outermost layer of the U slabs with different numbers of layers. For comparison, the theoretical values of Stojić *et al* [25] are presented. The magnetic moments are in units of μ_B.

	$S_{[GGA]}$	$S_{[GGA+SOC]}$	$L_{[GGA+SOC]}$	$Total_{[GGA+SOC]}$
1 L	2.871, 2.420[a]	2.971, 2.110[a]	−0.986, −0.830[a]	1.985, 2.010[a]
3 L	1.280	0.860, 0.840[a]	−0.320, −0.380[a]	0.540, 0.660[a]
5 L	1.279	0.859, 0.840[a]	−0.319, −0.380[a]	0.540, 0.650[a]
7 L	1.278	0.859, 0.840[a]	−0.319, −0.380[a]	0.540, 0.650[a]

[a] Reference [25].

the trend to the formation of the ferromagnetic ground state. If we assume that the Stoner parameter I estimated for U compounds [31] can be used to describe the free-standing U ML, the Stoner criterion is fulfilled. Indeed, the spin-polarized calculations result in a self-consistent ferromagnetic state with the total energy lower than the energy of the nonmagnetic state (see figure 2). The higher is the DOS at the Fermi level for the nonmagnetic ML (figure 2) the larger is the magnetic moment in the ferromagnetic state (figure 2).

In table 1, we collect the calculated values of spin (spin and orbital) magnetic moments for films consisting of 1 to 7 ML. For comparison, the results of the previous calculations [25] are presented. The magnetic moment per atom for the 1 ML film is large: 2.871 and 1.985 μ_B for the calculations with and without SOC. For thicker films, the calculated surface moment is stable with the change in the number of layers. This stability is explained by the fact that only the surface layers carry sizable magnetic moment. All other layers are very close to nonmagnetic, independent of the slab thickness. Our calculated magnetic moments are in the same range as in previous calculations [25].

The calculated magnetic moments for a free-standing U ML and for the surface layer of the 3 ML film are presented in figure 4 as a function of the lattice parameter. The magnetic moment decreases with decreasing atomic spacing.

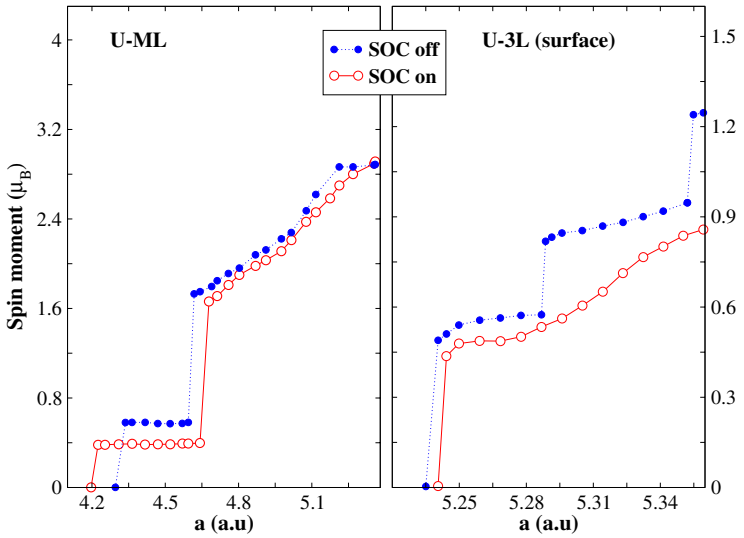

Figure 4. The magnetic moment as a function of the lattice constant for the 1 ML film and for the surface layer of the 3 ML film with and without SOC.

Table 2. The calculated MAE and Curie temperature for the 1 ML-film and surface layer of the 3 ML-film.

	Δ (mRyd/atom)	T_C^{RPA} (K)
1 ML	3.641	1184
3 ML	0.258	215

An interesting feature of the dependence of the magnetic moment on the lattice parameter is its discontinuous character. Such a behaviour can be explained by the presence of two minima of the total energy as a function of the magnetic moment. For larger lattice spacings the state with larger moment (high-moment state) has lower energy. With contraction of the lattice a critical lattice parameter is reached where both energy minima have equal values. With further lattice contraction the low-moment state becomes energetically preferable. Correspondingly a discontinuous transition from the high-moment state to the low-moment state takes place.

3.1.2. Exchange interactions and Curie temperature of U(001) surface. In figure 5, we present the calculated interatomic exchange parameters for the 1 ML film and for the surface layer of the 3, 5 and 7 ML films. In all cases the dominating exchange interactions are the ferromagnetic interactions with first and second nearest neighbours. The interactions with further neighbours are much weaker. The leading ferromagnetic exchange interaction in the 1 ML-film is much stronger than in the multiple-ML films. The magnetic anisotropy energy (MAE) is also much stronger in the 1 ML case (table 2). The MAE is calculated as the energy difference between the in-plane and out-of-plane orientations of the atomic moments. The preferable direction of the magnetic moments is orthogonal to the surface.

The calculated exchange parameters and MAE can be used for the estimation of the Curie temperature. In table 2 we present the calculated values of MAE and Curie temperature for 1 and 3 ML films. The value of T_c for the 1 ML film is about 5 times larger than for the 3 ML system.

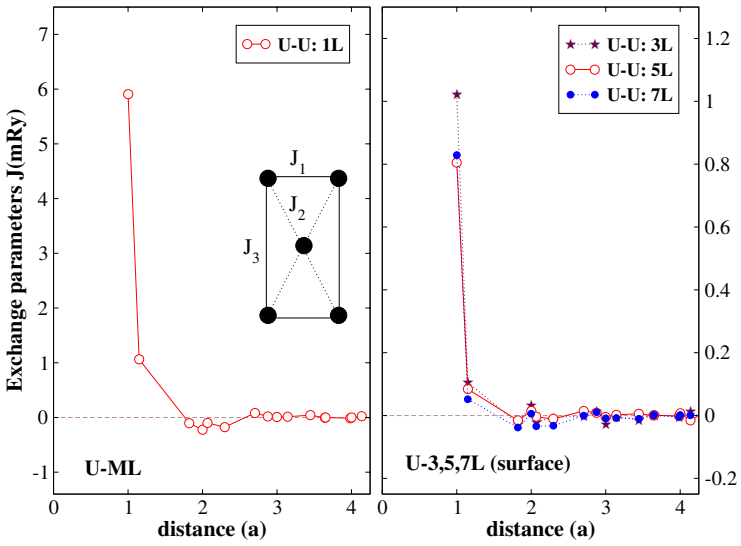

Figure 5. The exchange parameters for the atoms of the surface layer for films with 1, 3, 5 and 7 ML as a function of the inter-atomic distance. The distance is given in the units of the lattice constant.

Table 3. Calculated magnetic moments of $U(001)_1/Fe(110)_3$ multilayers. The scalar-relativistic calculation gives the value of the spin moment. In the fully-relativistic calculations both the spin and orbital moments are estimated. Fe_1 and Fe_3 correspond to the interface Fe layers, Fe_2 corresponds to the central layer. The magnetic moments are given in units of μ_B.

	$S_{[GGA]}$	$S_{[GGA+SOC]}$	$L_{[GGA+SOC]}$	$Total_{[GGA+SOC]}$
U	−0.930	−0.922	0.157	−0.765
Fe_1, Fe_3	1.400	1.340	0.050	1.390
Fe_2	2.658	2.641	0.076	2.717
U(001)[a]	1.660	1.246	−0.251	0.995

[a] $a_{Fe[110]}$

3.2. *Magnetism of* $U(001)_1/Fe(110)_3$ *multilayers*

In this section we discuss the first theoretical attempt to study the magnetism of the U/Fe multilayers. In table 3 we collect the values of the atomic magnetic moments. The spin moments of the Fe atoms belonging to different layers are parallel to each other. The U spin moments are antiparallel to the Fe moments. The atomic Fe moments in the interface Fe layers are somewhat reduced compared to bcc bulk Fe. On the other hand, the magnetic moment of the central layer is enhanced compared to the bulk value. For the same lattice constant, the spin magnetic moments at the U site in a free ML and multilayers are 1.66 and 0.93 μ_B, respectively. The relaxation of the lattice at the interface leads to a decrease of the magnitude of the magnetic moments of Fe and U at the interface.

The analysis of the DOS allows us to reveal the physical reason for the decrease of the U moments. In figure 6, the local DOSs for the U and Fe layers in $U(001)_1/Fe(110)_3$ multilayers are presented. For comparison, we show the DOS of a free-standing U ML with the lattice parameter used in the multilayer calculation and the DOS of the bulk bcc Fe. It is seen that the DOS of the central Fe layer is rather close to the DOS of the bulk bcc Fe. On the other hand,

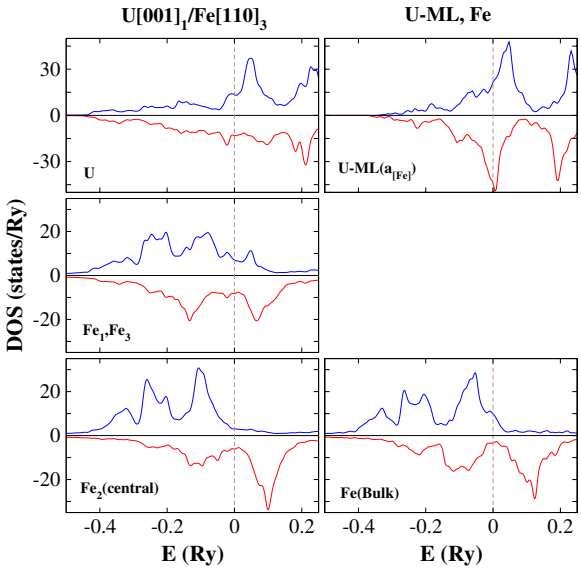

Figure 6. Local densities of states of U(001)/Fe(110) multilayers. The upper left panel corresponds to the U overlayer, and the upper right panel represents a free-standing U ML with the same lattice constant. The central left panel corresponds to the interfacial Fe layer ($Fe_1 = Fe_3$) and the bottom left panel to the central Fe layer. The bottom right panel shows the DOS of the bulk Fe. The vertical dashed line gives the position of the Fermi level.

the DOS of the interface layers deviates strongly from the bulk one. Also in the U DOS there is a strong difference between the free-standing U ML and the U ML in the multilayers. This difference is especially clearly seen in the spin-down channel. These differences in the DOS are the result of the strong U–Fe hybridization. Therefore the decrease of the moments of the interface layers is the consequence of the U–Fe hybridization.

The calculation of the magnetic anisotropy energy for the Fe/U multilayers shows that, similar to the case of U slabs, the easy axis is orthogonal to the layers. The energy difference between the in-plane and out-of-plane directions of the U moments is $\Delta = 0.248$ mRyd/atom.

In table 4 we present the contributions

$$J_0^{AB} \equiv \sum_{\substack{j \\ (jB)\neq(0A)}} J_{(0A),(jB)} \tag{6}$$

to the total exchange parameters at site $(0A)$ coming from the atoms of sublattice B. For diagonal elements ($A = B$) the main contribution comes from in-plane interactions. For off-diagonal elements ($A \neq B$) the main contribution is given by the nearest B planes.

The in-plane Fe–Fe and U–U interactions as well as the interactions between neighbouring Fe planes are strongly ferromagnetic, resulting in the ferromagnetism of the Fe layers. On the other hand, the Fe–U interactions are antiferromagnetic, leading to opposite directions of the Fe and U moments.

In figure 7, we present the calculated temperature dependence of magnetization. The calculations are based on the consideration of the Heisenberg Hamiltonian with exchange parameters obtained within the parameter-free DFT approach (section 2). The RPA method described in [36] was used. The spins were treated as classical vectors with values given in table 4. The calculated temperature dependences of the layer magnetizations are presented in figure 7. For Fe sublattices the curves have characteristic Langevin-type form. The temperature

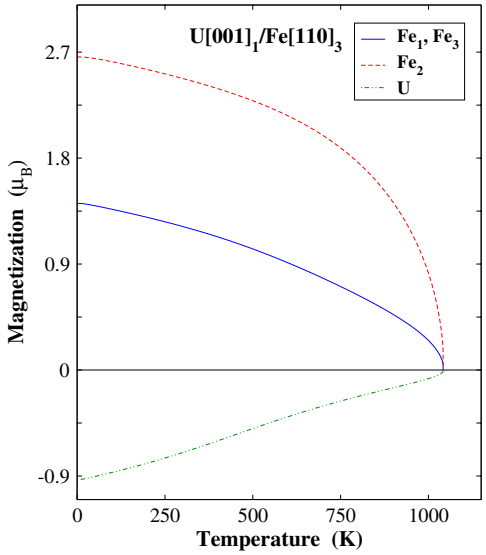

Figure 7. Temperature dependence of the layer magnetization for $U(001)_1/Fe(110)_3$.

Table 4. Calculated contributions J_0^{AB} (in mRyd) (equation (6)) to on-site exchange parameters for $U(001)_1/Fe(110)_3$ multilayers. For diagonal elements of the matrix ($A = B$) the sum in equation (6) includes contributions from the atoms of the plane where atom ($0A$) is situated and neighbouring planes of A type. The contribution of the in-plane interactions only is given in parentheses. For the off-diagonal elements of the matrix ($A \neq B$) the contribution of the nearest B planes only is considered.

$A\backslash B$	Fe_1	Fe_2	Fe_3	U
Fe_1	2.183 (2.207)	4.246	−0.037	−1.684
Fe_2		7.694 (7.753)	4.246	−0.261
Fe_3			2.183 (2.207)	−1.684
U				1.040 (1.040)

dependence of the U magnetization, however, deviates strongly from the Langevin form, which reflects the complexity of the exchange interactions in the system.

The Curie temperature T_C is obtained as the point where layer magnetizations vanish. The calculated value is 1043 K and it appears to be very close to the T_C value of bulk Fe. Recently, Beesley *et al* [26, 29] reported measurements of the Curie temperatures for U/Fe multilayers with different number of Fe and U layers. The measured values range from 477 to 634 K, which is considerably smaller than our value of 1043 K for $U(001)_1/Fe(110)_3$. The reason for the reduction of the experimental Curie temperature can be imperfectness of the Fe–U interfaces.

4. Conclusion

This paper presents the results of our comprehensive investigation of the magnetic and electronic properties of U surface and U(001)/Fe(110) multilayers within the framework of the parameter-free density functional theory. We report both scalar-relativistic and fully relativistic calculations. In agreement with previous calculation by Stojić *et al* we obtain the surface layer of the U films to be magnetic for the bulk lattice parameter. The dependence of the

magnetic properties of the U films on the lattice parameter was studied. It was shown that decreasing distances between U atoms lead to decreasing magnetic moment and finally to the nonmagnetic ground state. The variation of the magnetic moment as a function of the lattice parameter is discontinuous. Using the frozen-magnon approach we evaluated the parameters of the inter-atomic exchange interactions and estimated the Curie temperature. There is no experimental information on T_C available and our calculations are a prediction aiming to stimulate experimental studies.

We presented preliminarily results for U/Fe multilayers. Our calculations showed that for $U(001)_1/Fe(110)_3$ system the U layer is magnetic with the direction of the U moments opposite to the Fe moments. The importance of the U–Fe hybridization is revealed. Both the intra-layer (U–U, Fe–Fe) and inter-layer (U–Fe) exchange interactions were evaluated. The temperature dependence of the layer magnetization was studied within the random-phase approximation to the Heisenberg Hamiltonian of classical spins.

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