Magnetic structure of Fe/Cu(001) thin layers

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Ab-initio fully relativistic band structure calculations of Fe films on Cu (001) substrate are presented. The films are modelled as 6Cu/nFe/6Vc slabs, where the number of multilayers (ML) is n=1, 2, 4 and 6. Intermixing between Fe atoms of the thin film and the Cu atoms of the substrate was found to be energetically favourable for 1ML coverage, causing also a decrease of the Fe magnetic moment. The mixing of deposited Fe atoms with the Cu substrate has been studied using the Coherent Potential Approximation (CPA). Various ferromagnetic and ferrimagnetic spin configurations with coupling of layer blocks have been considered, with the in-plane and out-of-plane direction of magnetization. Total energy calculations have been performed and the most stable spin configuration for unrelaxed fcc thin films are shown. While for the 1 and 2 ML Fe/Cu(001) a ferromagnetic out-of-plane spin configuration is the most stable, 4 ML and 6 ML cover regimes exhibit a spin configuration with blocks of layers ferrimagnetically coupled. Layer-resolved spin and orbital magnetic moments in the ground state configuration have also been determined for 1, 2, 4 and 6 ML coverage.

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1. Introduction

Thin films and nanostructures show magnetic and electronic properties fundamental different compared with the corresponding bulk materials, allowing a large variation of coercitivity, magnetic anisotropy, magnetic moment and exchange coupling, magnetoresistance and many other properties. In the case of ultra-thin layers, the most important from the magnetic point of view is the dimensionality effect, the variation of the magnetic moments at surface and interfaces correlated with the magnetic anisotropy arising from low dimensionality due to surfaces and interfaces. Fe films epitaxially grown on a Cu (001) substrate is a subject of great interest for more than two decades. Thin films of Fe on Cu (100) show different types of magnetic ordering depending on the layer thickness. Under 4 ML (multilayer) (region I), the thin films show a ferromagnetic ordering having the Curie temperature higher than room temperature. Between 5 and 11 ML (reg. II), the ferromagnetic order appear just near the surface [1,2]. Although the image described before is generally accepted, some aspects concerning the magnetic ordering and the spin structure of the Fe/Cu(100) and Fe/Cu(111) films are still unclear. Whilst the ferromagnetic ordering has been established for Fe/Cu(100) in region I [3,4], the physical explanation is still under debate. In the latest studies, the ferromagnetism observed in Fe/Cu(100) films with a thickness under ML is related to the expanding of the atomic volume. The thin films in this region show an enhanced atomic volume compared with fcc Cu [5], favouring the appearance of higher magnetic moments compared with Fe bulk-ones. The magnetic properties of Fe/Cu(100) films in region II can be also be explain using this hypothesis. For these films, a fundamental antiferromagnetic state has been accepted by most of the studies [6-8]. Despite of that, the details of the antiferromagnetic configuration of spins and the Néel temperature are still unclear. H.-T. Jeng and D.-S. Wang discovered recently binary alloys of Fe-Co and Fe-Ni with a single layer, deposited on Cu, where a spin reorientation as a function of Fe concentration appears [9]. Concerning the thin films of Fe/Cu(100) in region II, their anomaly magnetic behaviour around 200 K should be mentioned. This behaviour has been observed first by Li et al. [10] in polar MOKE measurements. The magnetization saturation oscillates, with a peak separation of 2.6 ML in region II. A non-collinear spin structure has been excluded in order to explain this behaviour. Similar oscillations have been observed by Qian et al. [11]; they propose a density of spins with antiferromagnetic configuration to explain this behaviour. The anomaly magnetic behaviour has been observed also for others bi-layered structures containing layers of bcc Fe in region II (thickness between 5 and 11 ML), around 200K [12-14]. Sandratskii studied the fcc Fe/Cu(001) films with 6, 7 and 8 ML coverage and suggested a view on the magnetism of the Fe/Cu(001) films consisting in layers grouped into blocks with collinear magnetic structure [15], the coupling between blocks being ferrimagnetic. Also, it was demonstrated that the variation of the relative direction of the magnetization of different blocks is not relevant. For three surface layers, the magnetic structure has the form ↑↑↓ and further layers form pairs with robust ferrimagnetic structure. The formation of an incommensurate SDW in the thin films of Fe/Cu(001), suggested by Qian et al. [11] has been excluded by the studies of Sandratskii [15] and Amemiya et al.[16], proving instead a very strong variation of the magnetization from layer to layer without incommensurate periodicity.

In the present work, we investigate the magnetic ordering of Fe/Cu(001) films by fully relativistic band structure calculations. We considered Fe/Cu(001) films in fcc structure with the structure 6Cu/nFe/6Vc, where n=1, 2, 4,

6 is the multilayer (ML) number and Vc stands for the vacuum layers. The ground state spin structure is discussed, based on the total energy calculations. The intermixing of Fe atoms from the surface layer with Cu atoms of the substrate has been studied for 1 ML of Fe/Cu(001). Also, the variation of the Fe magnetic moments from layer to layer for the ground spin state and the influence of Fe-Cu intermixing on the magnetization are discussed in correlation with the previous investigations.

2. Computational details

The correlation between the structure and magnetism of the 3d metals thin layers has been investigated using the tight-binding-KKR (Korringa-Kohn-Rostoker) band structure calculation method [17,18]. The electronic structure was calculated in a fully relativistic mode, by solving the appropriate Dirac equation. We performed the electronic band structure calculations using the spin-polarized fully relativistic Korringa-Kohn-Rostoker (SPR-TB-KKR) method in the atomic spheres approximation (ASA), in ferromagnetic and antiferromagnetic spin configurations [18]. The local spin density approximation (LSDA) for the exchange-correlation energy using the Vosko, Wilk and Nusair (VWN) parameterization was used [19]. For the integration over the Brillouin zone, the special points method has been used [20]. For the surface Brillouin zones a regular k-mesh of 44×44x1 points was used which corresponds to 276 k-points in the irreducible part of the Brillouin zone. The coherent potential approximation (CPA) has been used to deal with Fe/Cu intermixing [21]. The energy convergence criterion and the CPA tolerance have been set both to the value of 10^{-5} Ry.

3. Results and discussions

While face centered cubic (fcc Fe) is a high-temperature phase, bulk Fe crystallizes in a body-centered cubic (bcc) with lattice constant a_{Fe}^{bcc}=2.87 Å. This lattice constant seems to be not compatible with the dimensions of face-centered (fcc) Cu substrate lattice (a_{Cu}^{fcc}=3.61 Å), but the experimental studies showed that the Fe layer with fcc structure would fit almost without mismatch the Cu(001) substrate (a_{Fe}^{fcc}=3.58 Å). The experimental studies showed that the face-centered phases of Fe can be stabilized by epitaxial growth on fcc substrate of Cu(001) up to about 10ML [7,22]. The fcc-layered system consisting of 6 layers of Cu, n layer of Fe and 6 layers of vacuum (6Cu/nFe/6Vc) with n =1,2,4 and 6 has been constructed in order to perform band structure calculations. The individual layer relaxation effects have been neglected.

For 1 ML of Fe on Cu(001), the equilibrium lattice parameter has been calculated from the total energy plot vs. lattice constant represented in Fig. 1. From this figure, the equilibrium lattice parameter for the system of 1ML Fe/Cu(001) has been established at 3.572 Å, lower than the bulk fcc Cu lattice constant (3.61 Å) but comparable with fcc Fe (3.58 Å). Considering the ferromagnetic spin configuration and using the calculated lattice parameter, ab-initio band structure calculations with the in plane and out-of-plane magnetization direction have been performed. The lowest total energy corresponds to out-of-plane orientation of the magnetization. The magnetic moments of Fe in the ground state spin configuration are m_s=2.66 μ_B and m_l = 0.075 μ_B, values which are higher than the corresponding values for bulk bcc-Fe and can be attributed to changed bonding numbers due to low dimensionality of the studied system.

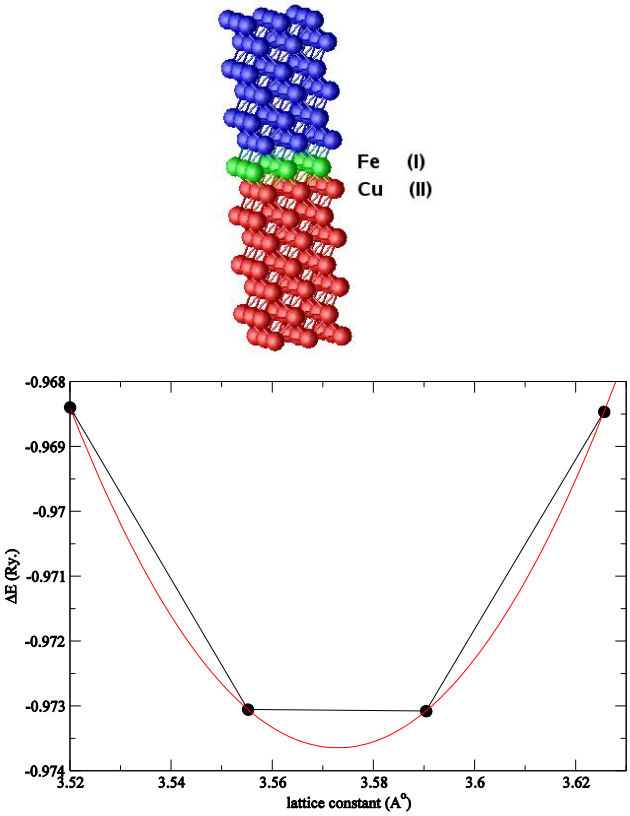

Fig 1. Left: The crystal structure of the layered fcc-6Cu/Fe/6Vc system. Right: The total energy vs. the lattice constant for 1ML Fe/Cu(001).

Fe and Cu, which are immiscible in equilibrium at room temperature and up to 600 °C [23], can nevertheless form mixed layers under sputtering conditions. The alloying effect has been evidenced by several experimental studies using different techniques [24-30]. The mixing of Fe and Cu at the interface has influence on the electronic and magnetic properties and the amount of mixing could change the magnetic moments magnitude due to the 3d-electron hybridization [31].

The mixing of the deposited Fe atoms with the substrate Cu atoms at the interface has been investigated. In the calculations, the mixing was limited at the 2 layers next to the surface (layers I and II in Fig. 1). To describe the mixing, a so-called mixing parameter x has been introduced, representing the percentage of Fe atoms moved into the Cu layer at the interface (with opposite movement of the Cu atoms).

The total energy vs. mixing parameter x is represented in Fig. 2, for both in-plane and out-of-plane magnetization

directions. In both cases, the lowest energy correspond to the mixing parameter x = 1, which means that the deposited Fe atoms on Cu (001) surface have the tendency to bury into the Cu interface layer.

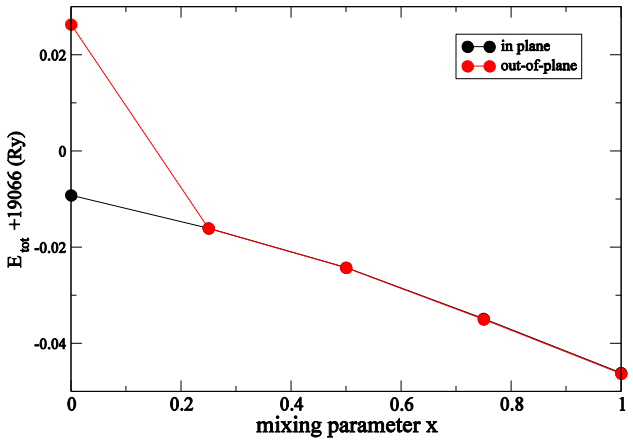

Fig. 2 The total energy vs. mixing parameter x for 1ML Fe/Cu(001) for the in-plane and out-of-plane magnetization directions.

The evolution of the Fe magnetic moments with mixing parameter is presented in Table 1. As can be seen in Table 1, the magnetic moments of the layered system decrease by increasing the mixing. As a consequence, by minimizing the energy of the system due to this mixing, the magnetic moments of the system are also minimized (m_s = 2.44 μ_B and m_l= 0.06 μ_B).

Table 1. The Fe magnetic moments evolution with mixing parameter x for the system 1ML Fe/Cu(001). (x is the concentration of the Fe atoms in layer II (see Fig. 1)). The total spin and orbital magnetic moments are calculated as weighted averages using the mixing parameter.

X		0	0.25	0.5	0.75	1.0
Fe I	m_s (μ_B)	2.66	2.68	2.69	2.69	
	m_l (μ_B)	0.07	0.09	0.1	0.1	
Fe II	m_s (μ_B)		2.29	2.35	2.40	2.42
	m_l (μ_B)		0.06	0.06	0.06	0.05
Total	m_s (μ_B)	2.66	2.61	2.55	2.51	2.44
	m_l (μ_B)	0.07	0.09	0.08	0.07	0.06

By increasing the coverage at 2ML of Fe/Cu(001), we obtained by optimization of the lattice parameter for the fcc-system 6Cu/2Fe/6Vc a lattice constant of a=3.56 Å, used to determine the ground magnetic state by further calculations. The total energy calculations performed considering the in-plane and out-of-plane magnetization directions, in ferromagnetic and ferrimagnetic configuration of the Fe spins are presented in Table 2. The lowest total energy is taken as reference. The calculations conclude that in the case of ideal structure (without mixing of atoms between layers) of 2 ML Fe/Cu(001), the ferromagnetic out-of-plane spin configuration is the most stable. The result agrees with previous studies [7,22] predicting ferromagnetic coupling of Fe layers in the region (I). We mention here the use of a fully relativistic calculation method, allowing for treatment of the spin polarization and spin-orbit coupling on an equal footing [32]. The spin-orbit coupling contribution at the magnetic anisotropy is taken into account and even if the 3d transition metals display poor spin-orbit coupling [33], the magnetic ground state can be determined with increased accuracy.

Table 2 Total energy difference for 2ML of Fe/Cu(001) in different spin state configurations. The lowest total energy is taken as reference.

ΔE_{tot} (mRy.)	out-of-plane	in-plane
FM	0	+0.3036
FERRIMAGNETIC	+10.5221	+10.7401

The magnetic moments of Fe in different spin configurations are shown in Table 3. At a coverage of 2ML Fe/Cu(001), we note the high spin moments of Fe (2.71 and 2.45 μ_B) of the most stable spin structure, which are much higher than the corresponding Fe bulk value (2.2 μ_B). Significantly smaller magnetic moments of Fe have been obtained for the ferrimagnetic spin structures with higher total energies.

Table 3 The magnetic moments of Fe atoms in 2 ML Fe/Cu(001) in different spin configurations. The Fe II atoms are in the layer next to the Cu (001) interface, whilst the Fe I atoms are in the layer next to the vacuum.

	FM				FERI			
	in plane		out of plane (ground state)		in plane		out of plane	
	m_s (μ_B)	m_l (μ_B)	m_s (μ_B)	m_l (μ_B)	m_s (μ_B)	m_l (μ_B)	m_s (μ_B)	m_l (μ_B)
Fe I	2.71	0.09	2.71	0.08	2.16	0.09	2.17	0.08
Fe II	2.45	0.065	2.45	0.07	2.08	0.06	2.08	0.06
total	5.16	0.16	5.23	0.16	0.08	0.03	0.09	0.02

Total energy calculations for 4ML of Fe/Cu(001) have been performed in several ferromagnetic and ferrimagnetic spin configurations. Several collinear spin configurations have been considered, denoted by the following sequence of arrows:↓↑↓↑, ↓↓↑↑, ↓↑↑↓ and ↑↓↑↑. Arrows are showing the spin orientation, from the layers next to substrate to the vacuum interface. The spin structures choice is based on the work of Sandratskii [15], where it was showed that the Fe layers are coupled into blocks with robust collinear structure. Also, Yavorsky et al. [34] showed that for 6Fe/8Cu/6Fe system built along [001] crystallographic direction, a collinear double layered antiferromagnetic structure is energetically favored. Several literature studies [10, 11, 35-37] prove that the upper two Fe layers are ferromagnetically coupled for the Fe/Cu(001) thin layer system, in the region I and II as defined by Meyerheim et al. [1]. The total energy variations with respect to the systems with lowest energy are shown

in Table 4 (for 4ML Fe) and Table 5 (for 6ML Fe), respectively.

Table 4 Total energy calculations for 4ML Fe/Cu(001) system in different spin configurations. Total energy variation is expressed in mRy.

ΔE_{tot} (mRy.)	out-of-plane	in-plane
FM	9.487	9.882
FERRIMAGNETIC ↓↑↓↑	9.125	15.146
FERRIMAGNETIC ↓↓↑↑	0.115	0.487
FERRIMAGNETIC ↓↑↑↓	12.15	10.586
FERRIMAGNETIC ↑↓↑↑	0	0.309

Table 5 Total energy calculations for 6ML Fe/Cu(001) system in different spin configurations. Total energy variations are expressed in mRy.

ΔE_{tot} (mRy.)	out-of-plane	in-plane
FM	13.968	9.115
FERRIMAGNETIC ↓↑↓↑↓↑	10.091	15.54
FERRIMAGNETIC ↑↑↓↓↑↑	0	0.292
FERRIMAGNETIC ↓↓↓↑↑↑	7.593	9.105
FERRIMAGNETIC ↑↓↑↓↑↑	7.954	0.655

In agreement with the previous studies [10,11,15,33], the most stable spin configuration for the 4ML of Fe/Cu(001) is an ferrimagnetic double layered structure, denoted as ↑↓↑↑, where the Fe layers next to the vacuum are ferromagnetic coupled. It should be noted that the second spin configuration having the last two layers ferromagnetically coupled, denoted as ↓↓↑↑ is energetically very close (at 0.115 mRy.) and can be easily compete with the ground state in the case of non-zero temperature. The same trend is followed by the system with higher Fe coverage, where blocks of Fe layers with ferrimagnetic coupling are the most stable.

In the case of the system with 6ML of Fe/Cu(001), the calculations show that the most stable is an out-of-plane configuration of spins denoted as ↓↓↑↑↓↓. This ground state spin configuration can be written as [↓↓↑][↑↓↓], evidencing the blocks of antiferromagnetically coupled layers, in agreement with the results of Sandratskii for 6ML system [15]. We should note that very close in energy is the in-plane configuration with the same sequence of spins.

We summarize our investigations by showing in Fig. 3 the Fe magnetic moments profiles in ground spin configurations for all 6Cu/nFe/6Vc system with n=1, 2, 4 and 6. As can be seen in Fig. 3, the spin magnetic moments of Fe are higher for the upper layer and for the layer next to Cu substrate, the intermediate layers having lower values of spin moments (even lower than bulk-Fe). The orbital magnetic moments follow the same trend as the spin moments, with the highest values next to the interfaces. One has to note also that the orbital magnetic moment is higher than the bulk value for each layer, in connection with distorted environment as compared with bulk.

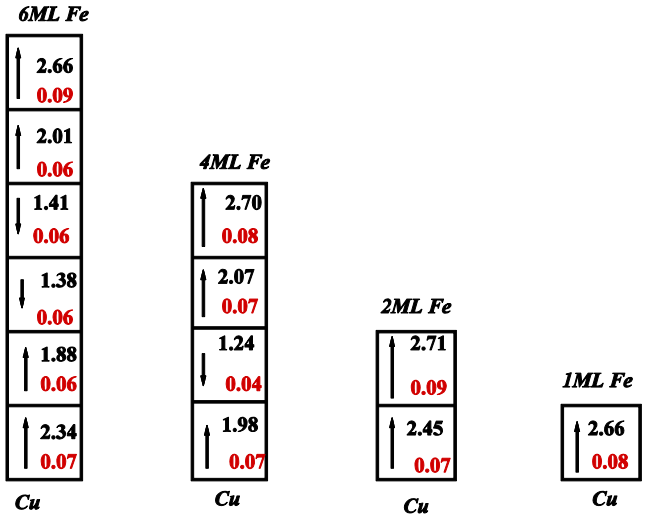

Fig 3. The magnetic profile of the fcc Fe/Cu (001) films with 1, 2, 4 and 6 ML coverage, obtained by SPR-KKR band structure calculations. The upper Fe layer is next to the Fe-vacuum interface. The values of spin (black) and orbital (red) magnetic moments are expressed in μ_B.

The study on the magnetic spin structure of Fe/Cu(001) with up to 6 ML of Fe presented here is in agreement with the theoretical and experimental studies, showing that the top layers are ferromagnetically coupled, while the deeper layers are characterized by nonferromagnetic ordering [6,10,11,36]. The previous studies of Meyerheim et al [38] using soft-x-ray resonant magnetic reflexivity (XRMR) experiments combined with first principle calculations, showed that the spin structure for 6 ML thick films can be written as [↑↑↓][↑↓][↑], from the top layer to the bottom (at the Fe/Cu interface). Our calculations indicate a similar spin structure, expressed as [↑↑↓][↓↑][↑]. Both calculations are using the same slab geometry, but different lattice parameters. Whilst the studies of Meyerheim et al. [38] use the lattice constant of an isotropic fcc-Fe film equal with the bulk Cu lattice constant, we determined an equilibrium lattice constant in our calculations. As the orientation of the spins of different blocks can vary easily [39] and the interblock interactions are relatively weak, small perturbations of crystal lattice or electronic structure can trigger transitions to different magnetic structures. At the origin of such dependence on the local coordination is the exchange-coupling interaction of Fe, which shows a strong dependence on the distance between neighbors. Further theoretical investigations for extended layer thickness, including all possible relaxations are needed to clarify the magnetic behavior of Fe/Cu(001) thin layers.

4. Conclusions

We presented fully relativistic band structure calculations of the total energies and magnetic moments for several types of collinear ferromagnetic and antiferromagnetic spin structures of ultrathin fcc Fe films grown on Cu(001) substrate. The systems were modelled as 6Cu/nFe/6Vc slabs (n = 1, 2, 4 and 6 ML). For 1 and 2 Fe ML, the preferred spin structure is ferromagnetic with out-of-plane magnetization. Among the considered magnetic structures, the ferrimagnetic coupling of layer blocks is energetically preferred for 4 and 6 Fe ML. The intermixing of Fe with Cu atoms of the substrate is favoured. The spin magnetic moments of Fe are higher (around 2.7 μ_B) for the upper layer close to vacuum and for the layer next to Cu substrate, whilst the spin moments of Fe from the intermediate layers are lower than bulk-Fe. The orbital magnetic moments of Fe are much higher than the bulk-ones, with the highest values next to the interfaces (about 0.08-0.09 μ_B near the vacuum interface).

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References

[1] H. L. Meyerheim, R. Popescu, D. Sander, J. Kirschner, O. Robach, and S. Ferrer, Phys. Rev. B **71**, 035409 (2005).
[2] C. A. F. Vaz, J. A. C. Bland and G. Lauhoff, Rep. Prog. Phys. **71**, 056501 (2008).
[3] J. Thomassen, F. May, B. Feldmann, M. Wutting, H. Ibach, Phys. Rev. Lett. **69**, 3831 (1992)
[4] R. D. Ellerbrock, A. Fuest, A. Schatz, W. Keune, R. A. Brand Phys. Rev. Lett. **74**, 3053 (1995)
[5] S. Müller, P. Bayer, C. Reischl, K. Heinz, B. Feldmann, et al., Rev. Lett. **74**, 765 (1995)
[6] R. E. Camley and D. Li, Phys Rev. Lett. **84,** 4709 (2000).
[7] L. Hammer, S. Müller, K. Heinz, Surf. Sci. **569,** 1 (2004).
[8] E. G. Moroni, G. Kresse, J. Hafner, J. Mag. Magn. Mater. **198-199,** 551 (1999).
[9] Horng-Tay Jeng, Ding-Sheng Wang, J. Mag. Magn. Mater. **317**, 46 (2007).
[10] Dongqi Li, M. Freitag, J. Pearson, Z. Q. Qiu, S. D. Bader, Phys. Rev. Lett. **72**, 3112 (1994)
[11] D. Qian, X. F. Jin, J. Barthel, M. Klaua, J. Kirschner, Phys. Rev. Lett. **87**, 227204 (2001)
[12] B. Schirmer, M. Wutting, Phys. Rev. B. **60**, 12945 (1999)
[13] Xiangdong Liu and Mattias Wutting, Phys. Rev. B. **64**, 104408 (2001)
[14] X. Liu, B. Schirmer and M. Wutting, Phys. Rev. B. **65**, 224413 (2002)
[15] L. M. Sandratskii, Phys. Rev. B **81,** 064417 (2010)
[16] K. Amemiya, S. Kitagawa, D. Matsumura, T. Yokoyama, T. Ohta, J. Phys.: Condens. Matter **15**, S561 (2003)
[17] R. Zeller et al., Phys. Rev. B **52**, 8807 (1995)
[18] H. Ebert, D. Koedderitzsch, J. Minar, Reports on Progress in Physics **74**, 096501 (2011).
[19] S. H. Vosko, L. Wilk, M. Nusair, Can. J. Phys. **58,** 1200 (1980).
[20] H. J. Monkhorst and J. D. Pack, Phys. Rev. B **13**, 5188 (1976).
[21] J.S. Faulkner, Prog. Mater. Sci. **27**, 1 (1982); J.S. Faulkner, G.M. Stocks, Phys. Rev. B **21,** 3222 (1980).
[22] P. Schmailzl, K. Schmidt, P. Bayer, R. Döll, K. Heinz, Surf. Sci. **312**, 73 (1994).
[23] Yavari A.R., Desre P.J., Benameur T. Phys Rev Lett. **68**, 2235 (1992).
[24] S.S.P. Parkin, N. More, K.P. Roche, Phys. Rev. Lett. **64,** 2304 (1990).
[25] D.H. Mosca, F. Petroff, A. Fert, P.A. Schroeder, W.P. Pratt Jr., R. Laloee, J. Magn. Magn. Mater. **94,** L1 (1991).
[26] S.S.P. Parkin, R. Bhadra, K.P. Roche, Phys. Rev. Lett. **66,** 2152 (1991).
[27] W.R. Bennett, W. Shwarzacher, W.F. Egelhoff Jr., Phys. Rev. Lett. **65** 3169 (1990).
[28] A.P. Kuprin, L. Cheng, D.W. Lee, Z. Altounian, D.H. Ryan, J. Appl. Phys. **85** 5738 (1999).
[29] A.P. Kuprin, L. Cheng, Z. Altounian, D.H. Ryan, J. Appl. Phys. **87,** 6591 (2000).
[30] D.W. Lee, D.H. Ryan, Z. Altounian, A.P. Kuprin, Phys. Rev. B **59** 7001 (1999).
[31] H. Choi, S.-C. Yi, Y.-C. Chung, Jpn. J. Appl. Phys. **47,** 5076 (2008).
[32] H. Ebert Electronic Structure and Physical Properties of Solids (Lecture Notes in Physics vol 535) ed H Dreyssé (Berlin: Springer) p 191 (2000).
[33] A.Enders, R.Skomski, J. Honolka J. Phys.: Condens. Matter. **22** 433001 (2010).
[34] B. Yu. Yavorsky, P. Zahn and I. Mertig, Phys. Rev. B **70,** 014413 (2004)
[35] J. Thomassen, F. May, B. Feldmann, M. Wuttig, H. Ibach, Phys. Rev. Lett. **69** 3831 (1992).
[36] T. Asada, S. Blügel, Phys. Rev. Lett. **79**, 507 (1997).; D. Spisak and J. Hafner, Phys. Rev. B **56,** 2646 (1997).
[37] Y. Zhou, L. Zhong, W. Zhang, and D-S. Wang, J. Appl. Phys. **81**, 4472 (1997).
[38] H. L. Meyerheim, J. M. Tonnerre, L. Sandratskii, H. C. N. Tolentino, M. Przybylski, Y. Gabi, F. Yldiz, X.I. Fu, E. Bontempi, S. Grenier, J. Kirschner, Phys. Rev. Lett. **103**, 267202 (2009).
[39] C. E. ViolBarbosa, H. L. Meyerheim, E. Jal, J.-M. Tonnerre, M. Przybylski, L. Sandratskii, F. Yldiz, U. Staub, J. Kirschner, Phys. Rev. B **85** 184414 (2012).

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