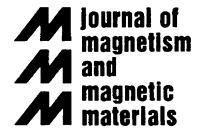




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Ab initio study of the magnetic configurations on the (001) surfaces of binary FePd and FeRh ordered alloys

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Abstract

Ab initio calculations of the local spin polarization at the (001) surfaces performed on the binary FePd and FeRh alloys are presented. For Rh-terminated FeRh (001) surface, the calculations indicate a possible magnetic reconstruction leading to a ferromagnetic order in the surface region, in contrast to the AF-II ground state of the infinite bulk FeRh alloy. © 2002 Elsevier Science B.V. All rights reserved.

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This work makes up continuity of studies done on the surface magnetic reconstructions of binary ordered alloys FeCr [1,2], and FeV [3] which exhibit interesting properties such as spin flip from an input magnetic order to another. FePd and FeRh alloys raised early interest as it has been shown that Pd and Rh become magnetically active with appreciable induced polarization such as in the presence of Fe impurities [4] or in Pd/Fe and Fe/Rh systems [5], [6]. Fe_{0.5}Pd_{0.5} as bulk or film [7] and FeRh thin films [8] has been extensively studied in recent years. A relevant point of general agreement is the strong Fe–Pd(Rh) ferromagnetic coupling. In this work, we use tight-binding linear muffin–tin orbital method developed in the atomic spheres approximations (TB-LMTO-ASA) [9,10], using the generalized gradient approximation (GGA) [11,12] and the local spin density (LSDA) [13] to determine the electronic structure and the local spin polarization of (001) surfaces of binary FePd and FeRh ordered alloys. We first studied the total energy as

function of the lattice parameter of bulk FePd in the CsCl and CuAu structures and bulk FeRh in the CsCl structure for different magnetic configurations. For FePd, the ground state is found to be ferromagnetic phase (FM) in the CuAu structure with an equilibrium lattice parameter of 7.12 ua. Following Moruzzi and Marcus [14,15], we have restricted, for FeRh, the study to the CsCl structure. In agreement with them, we have found that the ground state is of type II-antiferromagnetic (AF-II) with $a = 5.62$ ua. The FM and the AF-I states are, respectively, 1.1 and 1.73 mRy/atom higher in energy. Moreover, we have found an AF-III configuration at 7 mRy/atom above the ground state. One notices that the GGA reproduces better the experimental results than the LSDA; for this reason the next calculations were performed using only GGA approach.

The surface is modeled by repeated supercells made up of superposition of nine alternative metallic mono-layers of Fe and Rh (Pd) separated by five layers of atomic empty spheres. We use the interlayer distance obtained from total energy minimization of FePd (Rh) bulk alloys. The electronic and magnetic structures are calculated using 121 k -points in the first irreducible Brillouin Zone for both FeRh and FePd. We consider namely the possible $p(1 \times 1)\uparrow, p(1 \times 1)\downarrow$ and $c(2 \times 2)$

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magnetic configurations for either Fe or Rh(Pd) at the (001) surface.

The study of the relative stability among the $c(2 \times 2)$ and $p(1 \times 1)\uparrow(\downarrow)$ magnetic configurations for Fe at the (001) surface of Fe–Pd has shown that $p(1 \times 1)\uparrow$ order is more favorable. Indeed, the differences in energy $E\{p(1 \times 1)\downarrow\} - E\{p(1 \times 1)\uparrow\}$ and $E\{c(2 \times 2)\} - E\{p(1 \times 1)\uparrow\}$ are of 20.2 and 85.5 mRy, respectively (Fig. 1a). In this case, the Fe magnetic moment on the toplayer is equal to $3.03 \mu_B$ which corresponds to an increase of 3% in comparison with the bulk moment (Table 1) The same tendency is observed for the $p(1 \times 1)\downarrow$ solution, where the Fe moment reaches $-3.09 \mu_B$. Pd atoms at the subsurface (S-1) show a parallel spin polarization with a magnetic moment of $0.31 \mu_B$ when we consider $p(1 \times 1)\uparrow$ at the surface and go down to zero in the case of $p(1 \times 1)\downarrow$ order at the surface. The local magnetic moments on Fe atoms for the $c(2 \times 2)$ configuration are of 2.98 and $-3.04 \mu_B$ which gives nearly zero mean magnetic moment.

For Pd as toplayer, the ground state is similar to the case of Fe toplayer, i.e. the $p(1 \times 1)\uparrow$ is the lowest in energy. The difference in energy between the $p(1 \times 1)\uparrow$ order and, respectively, $p(1 \times 1)\downarrow$, $c(2 \times 2)$ is about 26 and 80 mRy. The magnetic moment on the Pd atoms in the different magnetic orders are $0.29 \mu_B$ for $p(1 \times 1)\uparrow$, $-0.29 \mu_B$ for $p(1 \times 1)\downarrow$ and $0 \mu_B$ for $c(2 \times 2)$ order. As we can see, no magnetic reconstruction is observed at the FePd (001) surface since Fe–Pd ferromagnetic coupling is conserved when going from the bulk to the (001) surface. We can explain the small increase of the Fe magnetic moment at the Fe toplayer and the decrease of the Pd moments in both cases of Fe or Pd toplayer by a strong hybridization between iron and palladium atoms.

In the present paper we have restricted the study of the magnetic orders at the surface of FeRh to the AF-II and FM states in the bulk. Indeed, for these two magnetic configurations, the slab thickness used is sufficient to recover the magnetic properties of the bulk (AF-II, FM) in the middle layer of the supercell. However, for AF-I, due to symmetry requirement, it is necessary to increase the slab thickness. This is under present investigations. As for FePd, we have considered the three input prefixed spin polarization: the two ferromagnetic orders $p(1 \times 1)\uparrow$, $p(1 \times 1)\downarrow$ and the $c(2 \times 2)$ in-plane antiferromagnetic solution at the (001) surface. In this case, contrary to the FePd (001) surface which stabilizes the $p(1 \times 1)\uparrow$ solution when Fe is the toplayer, here the $c(2 \times 2)$ solution is found to be the ground state (Fig. 1b). This result is qualitatively similar to those obtained at (001) surfaces of FeCr [1] and FeV [3]. The magnetic moment on Fe atoms at the surface is $3.16 \mu_B$ which corresponds to an enhancement of 2% compared to the bulk FeRh ($3.1 \mu_B$). Due to the symmetry of the $c(2 \times 2)$ spin orientation and to the

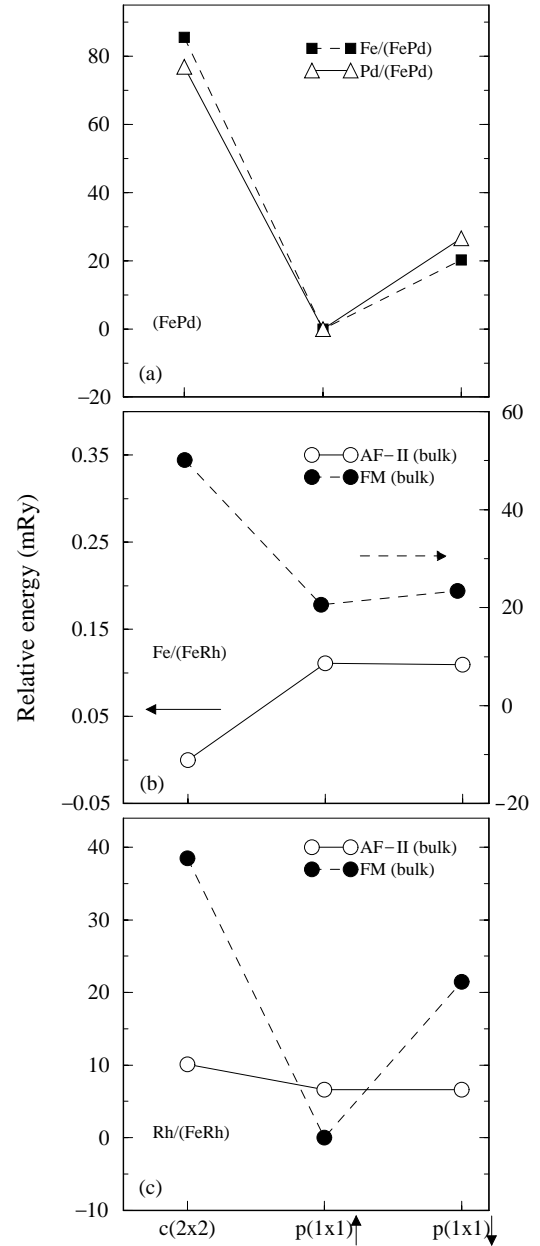


Fig. 1. Relative energy $E-E_0$ for the different magnetic configurations considered on the toplayer for: (a) Fe or Pd on FePd; (b) Fe on FeRh; and (c) Rh on FeRh (E_0 is the ground state energy).

ferromagnetic Fe–Rh coupling, no induced polarization on Rh layers (S-1), (S-3) is observed.

For the metastable ferromagnetic solutions $p(1 \times 1)\uparrow(\downarrow)$ on the Fe toplayer and AF-II configuration on the central layers, the Fe magnetic moment increases by 4%. The same magnetic solution at the surface is found to be stable at the (001) surface either in the FeCr [1]

Table 1

The magnetic moments distribution (in units of μ_B) on different atomic layers of FeRh (001) and FePd (001) surfaces for the most stable configurations

	Fe/FeRh $c(2 \times 2)$	Fe/FePd $p(1 \times 1)\uparrow$	Rh/FeRh $p(1 \times 1)\uparrow$	Pd/FePd $p(1 \times 1)\uparrow$
(S)	± 3.16	3.03	1.17	0.29
(S-1)	0.00	0.31	3.04	2.91
(S-2)	± 3.02	2.94	1.08	0.36
(S-3)	0.00	0.34	3.15	2.92
(S-4)	± 3.08	2.93	1.05	0.34

($m_{Fe} = 2.32 \mu_B$) or FeV [3] ($m_{Fe} = 2.35 \mu_B$). When we consider the FM orders ($p(1 \times 1)\uparrow$ and $p(1 \times 1)\downarrow$) on the toplayer with an AF-II configuration in the bulk alloy, it appears that there is an augmentation of 3% ($\pm 3.21 \mu_B$) as compared to the $\pm 3.1 \mu_B$ obtained in bulk FeRh which is of type AF-II configuration in the CsCl structure. Due to the strong Fe–Rh polarization, induced magnetic moments on Rh atoms at the subsurface layer (S-1) are obtained ($0.54 \mu_B$) for FM- $p(1 \times 1)\uparrow$ order considered at the surface. This spin polarization disappears on (S-3) Rh layer.

For Fe toplayer with FM alignment in the innerlayers, the Rh magnetic moments carried by (S-1) layer are 0.93, -0.1 and $0.36 \mu_B$ for, respectively, the $p(1 \times 1)\uparrow$, $p(1 \times 1)\downarrow$ and $c(2 \times 2)$ solutions on the top surface.

When Rh is the toplayer, the FM- $p(1 \times 1)\uparrow$ order at the surface and on both (S-1) and central layer (S-4) is energetically more stable (Fig. 1c). We observe an increase of the spin polarization on Rh atoms at the surface ($1.17 \mu_B$) compared to that obtained in the FeRh bulk ($1.05 \mu_B$) (11% increase in comparison with the corresponding bulk value). This result underlines clearly the effect of the surface perturbation namely the reduction of the coordination number and the apparition of surface states. Indeed, going from a quasi-degenerated magnetic configurations in the bulk FeRh, we obtain a FM alignment along the (001) direction.

In conclusion, we have performed an ab initio study of the magnetic reconstruction at the (001) surfaces of FePd and FeRh binary alloys. When the Rh is in the toplayer, the $p(1 \times 1)\uparrow$ order on the subsurface with a ferromagnetic phase in the bulk gives the lowest energy. The $c(2 \times 2)$ AF-II constitutes the most favorable state when the Fe is at the toplayer of FeRh. However, for either Fe or Pd in the toplayer of FePd, the most stable configuration is the $p(1 \times 1)\uparrow$ FM.

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