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# Ab initio study of the magnetic configurations on the (0 0 1) surfaces of binary FePd and FeRh ordered alloys

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**Abstract**

Ab initio calculations of the local spin polarization at the (0 0 1) surfaces performed on the binary FePd and FeRh alloys are presented. For Rh-terminated FeRh (0 0 1) 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 (0 0 1) 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 monolayers 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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