



Ab initio theory of transport in FeRh-based natural magnetic multilayers

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Abstract

The electronic structure and the residual resistivity of random FeRh-based alloys in the CsCl structure are calculated for different spin configurations using the tight-binding linear muffin–tin orbital method. The effect of substitutional impurities (Pd, Rh) is described by means of the coherent potential approximation. It is shown that impurity scattering leads to giant magnetoresistance effects in qualitative agreement with experiment. © 2002 Elsevier Science B.V. All rights reserved.

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A number of bulk intermetallic compounds consisting of alternating monolayers of magnetic and nonmagnetic atoms represent a simple model of magnetic multilayers. Such ‘natural’ magnetic multilayers often exhibit pronounced magnetotransport, magnetocaloric, and magnetovolume phenomena with a high application potential. A well-known example is the ordered FeRh alloy in the CsCl structure [1], where the monolayers of Fe and Rh atoms are stacked in the [001] direction. Its antiferromagnetic (AF) ground state can easily be changed to a ferromagnetic (FM) state due to elevated temperatures and/or applied magnetic fields whereby the phase transition is accompanied by a large drop in electrical resistivity [2] as well as by a large volume magnetostriction [3]. Similar properties were reported for off-stoichiometric FeRh alloys and for ternary Fe–Rh–TM systems where TM denotes a late transition-metal element (TM = Pd, Pt, Ni).

Recent ab initio theoretical studies of the FeRh system concentrated on the local magnetic moments, equilibrium volumes, and total energies of the FM and AF states [1,4] and on the effects of alloying by TM elements on the electronic structure [5,6]. The purpose of the present paper is to investigate the transport properties of the FeRh-based alloys from first principles in order to get (i) an explanation for the observed magnetoresistance effects and (ii) a relation to properties of magnetic multilayers [7]. We confined ourselves to calculations of residual resistivities for $\text{Fe}(\text{Rh}_{1-x}\text{Pd}_x)$ and $(\text{Fe}_{1-x}\text{Rh}_x)\text{Rh}$ systems ($0 \leq x \leq 0.2$), where the resistivity is due to substitutional randomness on one sublattice of the CsCl structure. Three different collinear spin structures were considered [4]: the FM state, the type-I AF state (AFI) with AF coupling between successive Fe(001) layers, and the type-II AF state (AFII) with AF coupling between successive Fe(111) layers which is the ground state of the stoichiometric FeRh compound.

The calculations were carried out using the self-consistent all-electron scalar-relativistic tight-binding linear muffin–tin orbital (TB-LMTO) method in the atomic sphere approximation (ASA) [8] combined with

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the coherent-potential approximation (CPA) for random alloys with atomic long-range order [9]. The lattice constant was fixed at the experimental value of the ordered FeRh compound for both systems and throughout the whole concentration range studied. Moreover, we neglected possible tetragonal distortions of the BCC lattice due to Pd alloying [5]. The diagonal elements of the conductivity tensor for electrons in a spin channel λ ($\lambda = \uparrow, \downarrow$) can be formulated in the Kubo linear-response theory neglecting the CPA vertex corrections as [10,11]

$$\sigma_{\mu\mu}^{\lambda} = -\frac{e^2}{\pi\hbar V_0 N} \text{Tr}\{\text{Im} \bar{g}^{\lambda}(E+i0)[X^{\mu}, S] \times \text{Im} \bar{g}^{\lambda}(E+i0)[X^{\mu}, S]\}, \quad (1)$$

where $\mu = x, y, z$ is the Euclidean index, V_0 is the volume of the primitive cell, N is the number of cells in a large but finite solid with three-dimensional periodic boundary conditions, the trace operation includes the site and orbital indices, $\bar{g}^{\lambda}(E+i0)$ is the configurationally averaged auxiliary Green function, E denotes the Fermi energy of the system, X^{μ} refers to the position operator, and S denotes the structure constant matrix of the TB-LMTO method. The residual resistivity is then equal to the inverse of the total conductivity $\sigma_{\mu\mu} = \sigma_{\mu\mu}^{\uparrow} + \sigma_{\mu\mu}^{\downarrow}$. The numerical evaluation of Eq. (1) is based on lattice Fourier transformations of the corresponding matrix quantities and a subsequent Brillouin-zone (BZ) integration. For example, the Fourier transform of the effective velocity operator $[X^{\mu}, S]$ is given by

$$[X^{\mu}, S]_{\mathbf{B}L, \mathbf{B}'L'}(\mathbf{k}) = \sum_{\mathbf{T}} (X_{\mathbf{B}}^{\mu} - X_{\mathbf{B}+\mathbf{T}}^{\mu}) S_{\mathbf{B}L, (\mathbf{B}+\mathbf{T})L'} \times \exp(i\mathbf{k} \cdot \mathbf{T}), \quad (2)$$

where \mathbf{B} denotes a basis (sublattice) vector, $L = (\ell, m)$ is the usual orbital index, \mathbf{k} is a vector in the BZ, \mathbf{T} denotes the translation vectors, and $X_{\mathbf{B}}^{\mu}$ is the μ th component of the vector \mathbf{B} . The BZ integration was performed using a uniform mesh of 8×10^6 \mathbf{k} -vectors.

The calculated electronic structures for the ordered stoichiometric FeRh alloy are in good agreement with previous results [1,4] regarding the densities of states (DOSs), the interatomic charge transfers and the local magnetic moments. The latter are equal to $M_{\text{Fe}} = 3.05 \mu_{\text{B}}$ and $M_{\text{Rh}} = 1.18 \mu_{\text{B}}$ for the FM state, while $M_{\text{Fe}} = 3.00 \mu_{\text{B}}$ and $M_{\text{Rh}} = 0 \mu_{\text{B}}$ in the AFI and AFII states.

The local Fe and Rh moments are only little sensitive to Pd alloying on the Rh sublattice. The Pd moment in the FM state of the $\text{Fe}(\text{Rh}_{1-x}\text{Pd}_x)$ alloy amounts to $0.4 \mu_{\text{B}}$ for $0 \leq x \leq 0.2$ and it exhibits an FM coupling to the Fe and Rh moments. The smaller exchange splitting of Pd atoms as compared to the Rh splitting leads to different strengths of disorder in the two spin channels: the majority ($\lambda = \uparrow$) electrons feel nearly no disorder in contrast to the minority ($\lambda = \downarrow$) channel with a sizeable

difference in the Pd and Rh potentials. This is manifested in the local DOSs: the majority of Pd and Rh DOSs are almost identical in the whole valence band, whereas a pronounced impurity peak appears in the minority Pd DOS at the Fermi level. As a consequence, the majority-spin conductivity in the FM state is much higher than the minority-spin one, which leads to much smaller resistivities in the FM state as compared to both AF states where no perfect matching of the Rh and Pd potentials can be found, see Fig. 1 [the conductivities are given in atomic units $e^2/(\pi\hbar a_0)$ where a_0 is the Bohr radius]. The tetragonal symmetry of the AFI state is reflected by two values of the conductivity: $\sigma_{xx} = \sigma_{yy}$ (the label AFIx in the figures) refers to a current in the (001) planes (CIP geometry) while σ_{zz} (the label AFIZ) refers to a current perpendicular to these planes (CPP geometry). A comparison of the corresponding resistivities (AFIx, AFIZ, FM) in Fig. 1 reveals that the CPP geometry leads to a bigger magnetoresistance effect than the CIP one similarly as in magnetic multilayers [7].

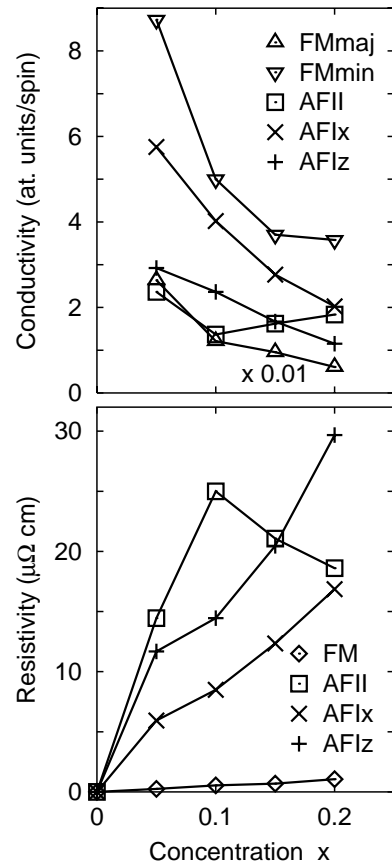


Fig. 1. The spin-resolved conductivities (top) and the total resistivities (bottom) for the FM, AFI and AFII states of $\text{Fe}(\text{Rh}_{1-x}\text{Pd}_x)$ alloys. The conductivity in the FM-majority channel was reduced by a factor of 100 in the plot.

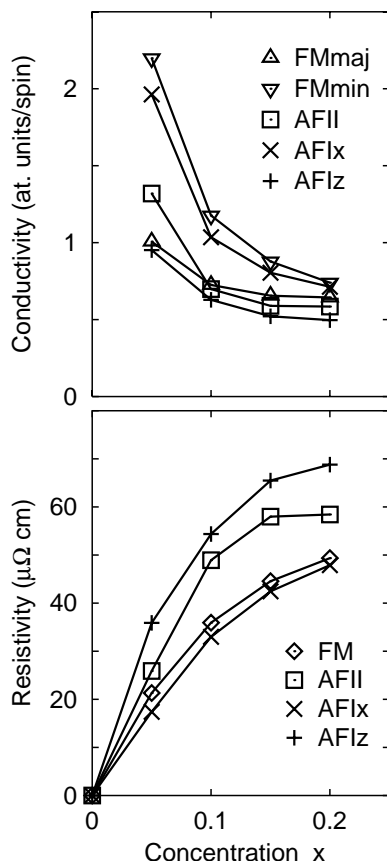


Fig. 2. The spin-resolved conductivities (top) and the total resistivities (bottom) for the FM, AFI and AFII states of $(\text{Fe}_{1-x}\text{Rh}_x)\text{Rh}$ alloys.

The results for the $(\text{Fe}_{1-x}\text{Rh}_x)\text{Rh}$ alloys are summarized in Fig. 2. The magnetoresistance effects are similar but much weaker as compared to the previous system. Quite surprisingly, the highest conductivity is found in the minority-spin channel in the FM state despite the fact that the Rh impurity is coupled ferromagnetically to the other two local moments and a small majority-spin disorder might be expected. However, the Rh-impurity moment (changing from 0.5 to $0.2 \mu_B$ for x going from 0 to 0.2) and its local exchange splitting are substantially

smaller than those of Fe atoms which leads to non-negligible diagonal (level) disorder in both spin channels. Moreover, the different localization of Fe-3d and Rh-4d orbitals induces additional off-diagonal (bandwidth) disorder which is strong and spin-independent. The higher minority conductivity then reflects the higher minority DOS at the Fermi level of the FeRh system in the FM state [4,6]. A detailed analysis of the AF conductivities has yet to be given. Nevertheless, the calculated relative decrease of the residual resistivity accompanying the AFII \rightarrow FM transition, varying between 16% and 27% (see Fig. 2), is in reasonable agreement with a 30% drop measured at the transition temperature $T_{tr} \approx 350$ K for a $\text{Fe}_{0.48}\text{Rh}_{0.52}$ alloy [2].

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