MAGNETISM IN FeRh ALLOYS

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We study the electronic and magnetic properties of FeRh ordered alloys. The electronic structure is calculated by the tight-binding linear muffin-tin orbital method. We observe the decreasing magnetic moment with increase of the ratio c/a during the structural phase transformation from CsCl to CuAu type structure.

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1. Introduction

The magnetic properties of $Fe_{1-c}Rh_c$ ordered and disordered alloys were studied in the last years [1–8]. Recently, Miyajima and Yuasa [2] have found that the fcc FeRh alloy was paramagnetic and stable at the room temperature. The change of bcc structure to a mixture phase composed of fcc and bct phases was performed by an application of uniaxial pressure of 2.5×10^4 kg/cm^2 to the bcc FeRh alloy. The experimental lattice constant for bcc FeRh alloy was $a = 2.981$ Å, and for the disordered fcc FeRh $a = 3.731$ Å. In the bct FeRh Miyajima and Yuasa [2] found $a = 2.81$ Å and $c = 3.38$ Å ($c/a = 1.203$). In this paper we study the change of the electronic structure and magnetic moment in FeRh ordered alloy during the structural transformation from the CsCl to CuAu type structure. The method of calculations is presented in Sec. 2 and the main results are discussed in Sec. 3. Finally we give some conclusions.

2. Method of calculations

The electronic structure and magnetic moment were calculated by the tight binding linear muffin-tin orbital (TB LMTO) method and the local spin density approximation (LSD) [9]. In the self-consistent band structure calculations we used the von Barth–Hedin [10] parametrization for the local exchange correlation potential. The values of the Wigner–Seitz radii were estimated from the minimum of the total energy. We find $S = 2.81$ a.u. in FeRh CsCl-type alloy. The main aim of this paper is an examination of the dependence of magnetic moment on ratio c/a during the structural transformation from CsCl to CuAu structure. We assume that the volume of the unit cell is constant. The lattice parameter a and the ratio c/a are changed in such a way to give the same volume of unit cell.

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3. Results

     We computed the band structure and magnetic moment in FeRh alloy for the different values of c/a $(1 < c/a < 1.41)$. In Fig. 1 we present the dependence of the total (FeRh) and local (Fe,Rh) magnetic moment on the ratio c/a. In the region $1.224 < c/a < 1.226$ we find the structural phase transition from
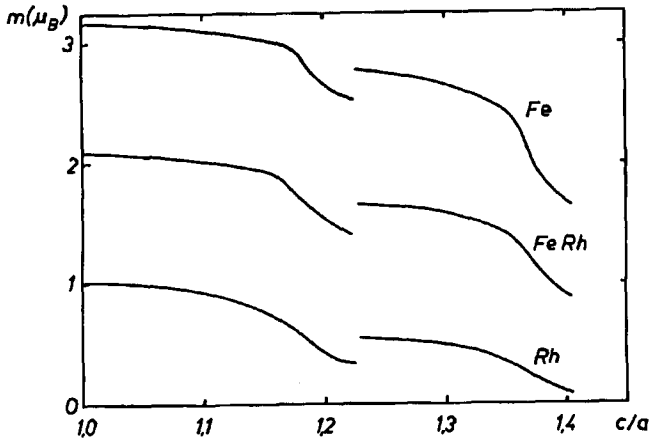

Fig. 1. The n n e of the total and local magnetic moment in FeRh on the ratio c/a.
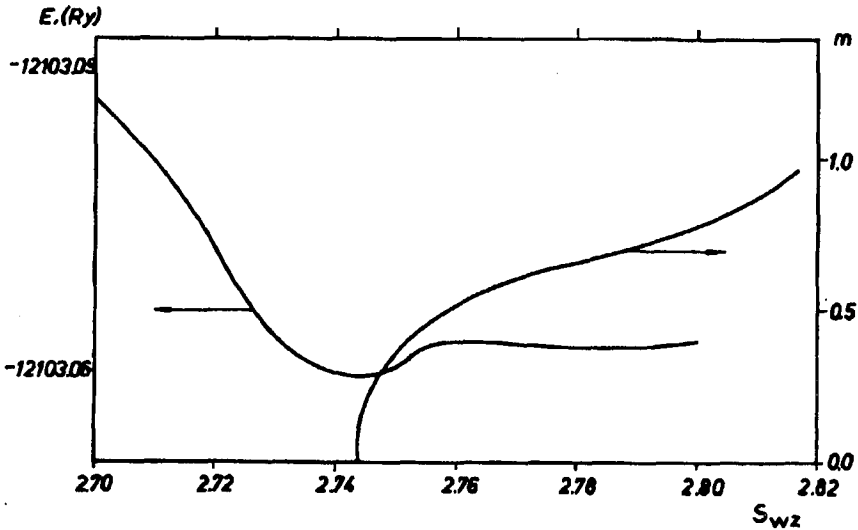

Fig. 2. The plot of total magnetic moment and the total energy versus the Wigner–Seitz radius.

bct to fct structure. The magnetic moment decreases with increase c/a, and for $c/a = 1.41$ the total magnetic moment for FeRh (CuAu) goes to 0.87 μ_B. Then we examine the energetic stability of FeRh (CuAu). In Fig. 2 we present the change of the total magnetic moment and the total energy versus the Wigner–Seitz radius. The total magnetic moment goes to zero for $S = 2.757$ a.u. For this value of S the system has the minimum of the total energy. The results obtained in this paper are in good agreement with the TB LMTO coherent potential approximation (CPA) results obtained by Jezierski [6]. Recently Jezierski has shown [6] that the fcc disordered FeRh alloys do not satisfy the Stoner criterion. The similar structural transition was observed by Krasko and Olson during the bcc–fcc lattice deformation in iron [11].

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