Vol. 97 (2000) *ACTA PHYSICA POLONICA A* No. 3

Proceedings of the European Conference "Physics of Magnetism '99", Poznań 1999

THEORETICAL STUDY OF PHASE DIAGRAMS FOR REENTRANT SUPERCONDUCTING $Er_{1-x}Ho_xX$, $Er_{1-x}Gd_xX$, $Er_{1-x}Tm_xX$, $Ho_xLu_{1-x}X$, AND $Sm_{1-x}Er_xX$ (X = Rh_4B_4) ALLOYS

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We consider a simplified version of the $s-f$ model, supplemented by the intersite Cooper pairs interaction between conduction electrons with opposite spins to investigate ferromagnetic and superconducting properties of an alloy $Re^{(1)}_{1-x}Re^{(2)}_xX$ ($Re^{(1),(2)}$ — rare earth elements, X = Rh_4B_4) using the virtual crystal approximation. For a suitable choice of the model parameters we can reproduce the phase boundaries of the experimentally measured phase diagrams for $Er_{1-x}Ho_xX$, $Er_{1-x}Gd_xX$, $Er_{1-x}Tm_xX$, $Ho_xLu_{1-x}X$, and $Sm_{1-x}Er_xX$ alloys.

PACS numbers: 75.30.Kz, 75.40.Cx

The alloy family $Er_{1-x}Ho_xX$, $Er_{1-x}Gd_xX$, $Er_{1-x}Tm_xX$, $Ho_xLu_{1-x}X$, and $Sm_{1-x}Er_xX$ (X = Rh_4B_4) exhibits very interesting properties, changing with the concentration x (cf. e.g. Ref. [1] and the papers cited therein). The whole alloy family possesses very similar crystalline and electronic structure (see [1, 2]). This advantage allows the use of the $s-f$ model with intersite Cooper pairs interaction described in Ref. [3]. This model, applied to the mentioned alloy family (VCA approximation [4]) with the use of a suitable model parameter set is able to reproduce all phase boundaries in the phase diagrams separating different phases of these alloys in quantitative agreement with experimental results [5–11]. To describe the properties of a $Re^{(1)}_{1-x}Re^{(2)}_xX$ alloy we start with a model Hamiltonian (see Ref. [3]) for ReX compound (grand canonical ensemble)

$$\overline{H}_{\mathrm{ReX}} = H_H + H_e + H_{l-e} + H_s - \mu N, \tag{1}$$

where

$$H_H = -\frac{1}{2}\sum_{i,j} K_{i,j}\boldsymbol{J}_i \cdot \boldsymbol{J}_j, \tag{2}$$

$$H_e = t_0 \sum_{i,\sigma} n_{i,\sigma} + \sum_{i\neq j,\sigma} t_{i,j} c^+_{i,\sigma} c_{j,\sigma}, \tag{3}$$

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$$H_{l-e} = -\frac{g}{2}\sum_i \left[J_i^+ c_{i,\downarrow}^+ c_{i,\uparrow} + J_i^- c_{i,\uparrow}^+ c_{i,\downarrow} + J_i^z \left(n_{i,\uparrow} - n_{i,\downarrow}\right)\right], \tag{4}$$

$$H_s = \sum_{i,j} R_{i,j} c_{i,\uparrow}^+ c_{j,\downarrow}^+ c_{j,\downarrow} c_{i,\uparrow}, \tag{5}$$

$$N = \sum_{i,\sigma} n_{i,\sigma}, \tag{6}$$

and μ is the chemical potential. The model Hamiltonian contains the following model parameters: $K_{i,j}$ (exchange integral between neighbouring $4f$-ions ($K_0 = \sum_j K_{i,j}$); see (2)), t_0 (center of gravity of the "effective" conduction band), $t_{i,j}$ (hopping integral; see (3)), g ($s-f$ coupling constant; see (4)), and $R_{i,j}$ (intersite Cooper pairing interaction parameter ($R = R_{i,j}$, i,j — n.n.); see (5)). To derive the corresponding Hamiltonian for the $\mathrm{Re}^{(1)}_{1-x}\mathrm{Re}^{(2)}_x\mathrm{X}$ alloy we first apply the mean field approximation (cf. also [3]) to the Hamiltonian (1). In the virtual crystal approximation (VCA) the Hamiltonian of the alloy (cf. e.g. [4]) can be written in the form

$$\overline{H}_{\mathrm{Re}^{(1)}_{1-x}\mathrm{Re}^{(2)}_x\mathrm{X}} = (1-x)\overline{H}_{\mathrm{Re}^{(1)}\mathrm{X}} + x\overline{H}_{\mathrm{Re}^{(2)}\mathrm{X}}, \tag{7}$$

$$n = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle, \tag{8}$$

where n is a given average number of electrons per magnetic ion which should be constant for the whole family of the alloys. The parameter set of the alloy can be divided into two partial parameter sets, corresponding to the limiting cases $x = 0$ ($\mathrm{Re}^{(1)}\mathrm{X}$ compound) and $x = 1$ ($\mathrm{Re}^{(2)}\mathrm{X}$ compound). Such quantities as n (see (8)), the partial band widths $W^{(1,2)}$, and other parameters can be deduced from [12]. The practical calculations were performed with the use of a true density of states for the fcc lattice (the Jelitto formula). The calculated phase boundaries of the whole alloy family in comparison with experimental results are presented in Fig. 1. The quantitative agreement of the calculated and experimentally measured phase diagrams (Fig. 1) clearly indicates that the mechanism of the chemical binding in these alloys, depending on the concentration x, realizes in a good approximation the VCA scheme of averaging over the alloy configurations in the whole interval of $x \in [0,1]$.

There are, however, still open questions concerning the type of the magnetic ordering in the magnetic phase. The starting point of the VCA model (7) was the assumption that the value of the total angular momentum J, connected with the $4f$-shell of the particular Re^{3+} ion in the alloy is equal to its free ion value (we have neglected the influence of the crystal field effects). As a consequence of this assumption we have obtained only one ferromagnetic phase in the phase diagrams. The nature of the magnetic ordering in the real alloys is, however, much more complicated and depends on the concentration x (see [5–11]). In reality, in Fig. 1a the magnetic phase (see [6]) is ferromagnetic for $x \in [0.3, 1]$, for very small temperatures is mixed ferromagnetic, and sinusoidally modulated with small overlap with superconducting phase for small concentrations. According to Ref. [7], this

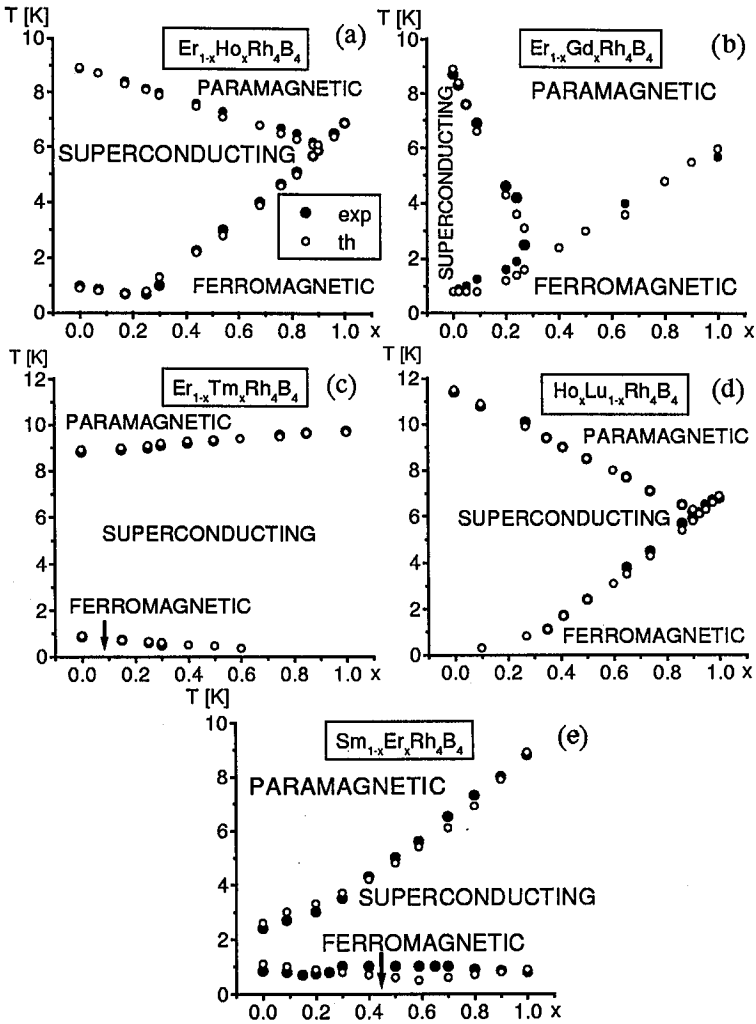

Fig. 1. Calculated phase diagrams (open circles) in comparison with experimental points (filled circles) from Ref. [5] (a), Ref. [10] (b), Ref. [7] (c), Ref. [11] (d) and Ref. [9] (e). Partial parameter set for $ErRh_4B_4$ (common for (a,b,c,e)): $t_0 = 0$, $W = 0.5$ eV, $g = 0.0007$ eV, $K_0 = 0.0000033$ eV, $R = 0.071$ eV, $J = 15/2$; for $HoRh_4B_4$ (common for (a, d)): $t_0 = 0$, $W = 0.48$ eV, $g = 0.0062$ eV, $K_0 = 0.0000106$ eV, $R = 0.0635$ eV, $J = 8$; for $GdRh_4B_4$ (b): $t_0 = 0$, $W = 0.48$ eV, $g = 0.003$ eV, $K_0 = 0.00095$ eV, $R = 0.026$ eV, $J = 7/2$; for $TmRh_4B_4$ (c): $t_0 = 0$, $W = 0.55$ eV, $g = 0.001$ eV, $K_0 = 0.000001$ eV, $R = 0.078$ eV, $J = 6$; for $LuRh_4B_4$ (d): $t_0 = 0$, $W = 0.65$ eV, $g = 0$, $K_0 = 0$, $R = 0.0921$ eV, $J = 0$; and for $SmRh_4B_4$ (e): $t_0 = 0$, $W = 0.7$ eV, $g = 0.001$ eV, $K_0 = 0.0003$ eV, $R = 0.077$ eV, $J = 5/2$.

behaviour seems to be a typical crystal field effect. The calculations in Ref. [7], however, were performed only for the magnetic phase without considering the interference with superconductivity. The nature of the magnetic phase in Fig. 1b was

investigated in Ref. [8]. Ferromagnetic ordering was found for $x > 0.28$. In reality, in Fig. 1c the magnetic phase is of Ruderman–Kittel–Kasuya–Yoshida (RKKY) type (Ref. [7]). The magnetic phase in the phase diagram in Fig. 1d is formed by the effect of dilution of the magnetic Ho ions with non-magnetic Lu ions with decreasing x. The nature of this phase is probably ferromagnetic (see Ref. [9]). For small concentrations x in the case of the phase diagram presented in Fig. 1e the antiferromagnetic phase coexists with superconductivity, above $x > 0.15$ the magnetic phase is ordered ferromagnetically (see Ref. [9]).

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