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ELECTRONIC STRUCTURE AND ELECTRON-TRANSPORT PROPERTIES OF $(Gd_{1-x}Y_x)_2In$ COMPOUNDS

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Based on the electronic structure of the ferromagnetic Gd_2In and $(Gd_{0.5}Y_{0.5})_2In$ compounds the high-temperature magnetic part of the electrical resistivity of $(Gd_{1-x}Y_x)_2In$ as a function of Y concentration was calculated and analyzed. The main interaction which causes the finite magnetic part of the conductivity was assumed in a form of stochastically distributed in space $s-f$ interaction. The calculated resistivity of $(Gd_{1-x}Y_x)_2In$ alloys qualitatively reproduces the experimental data.

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1. Introduction

The $(Gd_{1-x}Y_x)_2In$ compounds were widely studied experimentally with the use of different methods and a variety of magnetic properties was reported for them (see Ref. [1] and references therein). For samples with around 15% of yttrium the effective magnetic moment reaches the maximum value and magnetic susceptibility shows the minimum. The resistivity measurements at temperatures below 100 K revealed the magnetic transitions for Y concentrations $x < 0.15$, while the saturation resistivity reaches the maximum at about $x = 0.15$. In our earlier paper [2] we have discussed already the most important results of the TB–LMTO [3] band structure calculations of the $(Gd_{1-x}Y_x)_2In$ compounds. The method description and the parameters used in the band structure calculations were also presented there. The calculated properties of $(Gd_{1-x}Y_x)_2In$ confirm the experimental observations. The density of states (DOS) around the Fermi level (ε_F) composed of mainly d-states of Gd and Y atoms displays a similar behavior as that observed by XPS measurements. In the present paper we resume the relevance of the resistivity calculations results of band structure investigations and report the calculations of the saturation electrical resistivity of the $(Gd_{1-x}Y_x)_2In$ compounds in the concentration range $x = 0.0 \div 0.5$.

2. Calculations and results

In order to calculate the electrical resistivity it is important to know the changes of the DOS structure (the shape and positions of the peaks) around the ε_F upon alloying. Figure 1 presents the summed s, p, and d DOS of Gd_2In and $(Gd_{0.5}Y_{0.5})_2In$. The analysis of the complete DOS has shown that the $4f$-minority--band of Gd atoms which lies above the Fermi level does not contribute significantly to DOS below and at ε_F. The influence of $4f$ levels on the electrical transport is mainly due to scattering of the conduction electrons on the localized spins of Gd atoms and to some extent due to the hybridization of minority $4f$-band states with *spd*-states which modifies the shape and position of *spd*-DOS around the ε_F. The analysis of Fig. 1 shows that the replacement of Gd with isoelectronic Y atoms removes the sharp peak of d-DOS from below the ε_F, broadens and shifts the d-states DOS around the ε_F to higher energies.

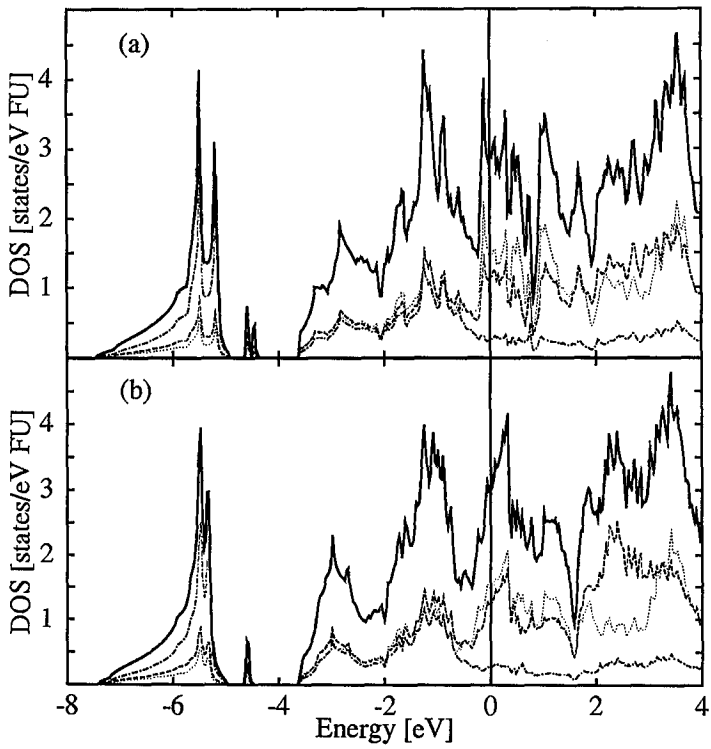

Fig. 1. The summed *spd*-density of states of Gd_2In (a) and $(Gd_{0.5}Y_{0.5})_2In$ (b). The dash-dot and dot lines represent the contributions from In and Gd_{2a} atoms, the dash lines show the contribution of Gd_{2d} (a) and Y_{2d} (b) (2a and 2d stand for the positions in the unit cell). The solid vertical line indicates the Fermi level.

To calculate spin disorder resistivity for the compounds it is necessary to know the structure of the lowest excited states which is not available within the ground-state TB–LMTO approach. Therefore we apply the well-known structure

of scattering levels for the Gd alloys at high temperatures [4–6]. In the case of $(Gd_{1-x}Y_x)_2In$ alloys we assume that for the static electrical resistivity (only the spin disorder resistivity part is discussed) two kinds of scattering mechanism are crucial. The first one comes from Gd atoms in the lattice. The Gd high spins (7/2, Hund's rule) cause the scattering mainly via $s-f$ interactions represented by the second term of Hamiltonian in Eq. (1). The second mechanism is the scattering due to the impurity Y atoms which have the atomic levels slightly shifted when compared with host Gd_2In levels. Assuming the completely disordered distribution of Y atoms and the case of high temperature we can apply the formalism of coherent potential approximation (CPA) to obtain the quasiparticle structure and DC electrical resistivity. Within the considered model, only one band undergoes the scattering. The many-body alloy Hamiltonian takes the form

$$H = \sum_{i,j,\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} - g \sum_{i\sigma} \xi_i s_i \cdot \boldsymbol{S}_i, \tag{1}$$

where s_i and $\boldsymbol{S}_i$ stand for the conducting electron and Gd-4f spins, respectively. Classical stochastic variable ξ_i takes the values 1 or 0, when the lattice site $\boldsymbol{R}_i$ is occupied by Gd or Y atoms, respectively. The hopping integral t_{ij} also depends on substitutional disorder and following Shiba [7] we assumed that t_{ij} satisfies the relation $t_{Gd,Y} = (t_{Gd,Gd} \cdot t_{Y,Y})^{1/2}$. Using the approach proposed by Rangete et al. [4] the complicated many-body problem involved in (1) was projected onto the simpler one-body problem. The resulting Hamiltonian is

$$H = \sum_{i,j,\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} + \sum_{i\sigma} E_i, \tag{2}$$

where the stochastic variable E_i at the site $\boldsymbol{R}_i$ takes the values $V_{Gd} - gS/(2S+1)$, $V_{Gd} + g(S+1)/(2S+1)$, and V_Y with the probabilities $(1-x)S/(2S+1)$, $(1-x)(S+1)/(2S+1)$, and x, respectively [8]. For the one-body alloy Hamiltonian (2) the CPA procedure was applied. Having the projected *spd* TB–LMTO DOS lying closely to the Fermi level E_F we have approximated the model DOS in that region by the triangle DOS shapes. Slightly different band-widths and the positions of the band centers of gravity (V_{Gd}, V_Y) for Gd_2In and $(Gd_{0.5}Y_{0.5})_2In$ conducting electrons were assumed. According to the TB–LMTO results the average number of the electrons responsible for the electric transport is about one half. Using the realistic value for the $s-f$ coupling constant g we have calculated the saturation spin disorder resistivity as a function of Y concentration. Figure 2 presents the results of calculations together with the available experimental data [1].

The calculated resistivity agrees with the experimental one satisfactorily even though we have not fitted the values of the model parameters in order to achieve the best agreement. From the TB–LMTO calculations the positions of the effective atomic levels V_{Gd}, V_Y, and widths of the electronic bands λ_{Gd}, λ_Y located very closely to the Fermi level were estimated. The exchange coupling constant g was taken positive with the realistic for the Gd-compounds value of magnitude. The detailed values are listed in the description of Fig. 2. From the results (Fig. 2) it is possible to recognize the mechanism of the scattering. For the high concentration of the Gd atoms ($x \ll 1$) the scattering on the different atomic levels is rather small. When the concentration x increases the scattering on atomic Gd spins becomes less

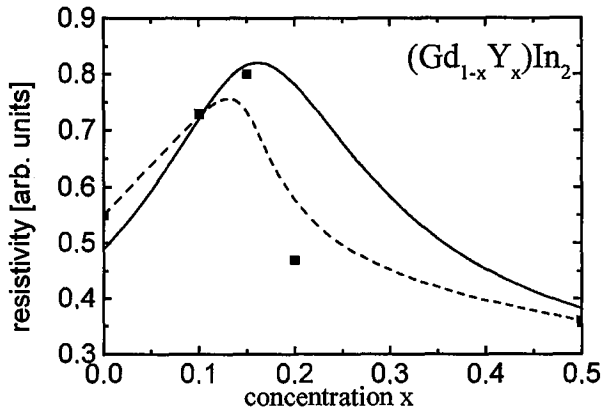

Fig. 2. Saturation of the spin disorder resistivity [arb. units] versus concentration of Y atoms. The continuous line shows the calculated results obtained for the following model parameters: $g = 0.007$ eV, $V_{Gd} = 0.007$ eV, $V_Y = 0.02$ eV, the base half-bandwidth = 1.0 eV and the bandwidths factors $\lambda_{Gd} = 0.1$, $\lambda_Y = 0.2$. The dash line is a spline of the experimental points (black squares).

important and at the same time drastically increases the resistivity part due to the atomic scattering. There is the value of concentration x for which the resistivity reaches the maximum. Simultaneously with decreasing number of Gd atoms the system becomes uniform again and the effect of the atomic scattering becomes less important. In order to get much better agreement between calculated and measured resistivities one should use the model in which the influence of chemical disorder on the band structure closely to the Fermi level is more accurately taken into account (e.g. KKR–CPA approach of Banhart et al. [9]).

Acknowledgments

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