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RESISTIVITY OF $(Gd_{1-x}Y_x)_2In$ ALLOYS AT HIGH TEMPERATURES — TWO-BAND MODEL APPROACH

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Two-band model for the substitutionary binary alloy of different rare earth metals with relatively simple $4f$ multiplet structure placed within the transition metal host matrix was proposed and applied to $(Gd_{1-x}Y_x)_2In$. The main interaction which causes the magnetic part of the resistivity was assumed in a form of stochastically distributed in space $s-f$ interaction. The calculated high temperature spin disorder resistivity of $(Gd_{1-x}Y_x)_2In$ alloys reproduces well the experimental alloys data.

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We have tried to describe the simple transport properties (dc resistivity and the thermoelectric power) of the binary $(R_xR'_{1-x})_nTM$ disordered rare earth (RE) alloys at high temperatures. The R, R', and TM denote the atoms of RE elements and transition metals, respectively. For the simplicity we have considered only the RE elements for which $4f$ electrons form relatively simple multiplets. Therefore we will deal with a disordered alloy which contains Y, Gd components. The transition metals element TM can be of any from the $3d$, $4d$ series which generates a stable disordered alloy with a relatively wide range of the concentrations of x. The magnitude of the local spin which relatively accurately describes the $4f$ shell properties was in our case 0, 7/2 $\hbar$. The influence of the orbital moment of the $4f$ shell was ignored. The modeling and the measurements of the dc resistivity for the RE pure metals and alloys have a long history. It was originated in the decade of 60th by the authors of [1–3] and was described there in many details. The presented models fit qualitatively to experimental resistivity results especially for the simple pure RE metals only.

Basing on the calculations of the electronic structure and analysis of the single particle spectrum near the Fermi energy E_F for the simplest $(R_xR'_{1-x})_nTM$ compounds ($x = 0$, 1/2, or 1 for example) it was possible to distinguish the partial bands which may contribute to the transport properties. We assume that two

different bands contribute to the electrical currents. One of them undergoes the strong scattering processes on the localized $4f$ spins and the second only hybridizes with the first one. The positions of the centers of gravity on the energy scale were also established from the one particle spectrum.

The many-body alloy model Hamiltonian which approximately describes the properties of the system specified above has the following form:

$$H = \sum_{i,j,\sigma}{}' t_{ij}^{(c)} c_{i\sigma}^{+} c_{j\sigma} + \sum_{i,\sigma} V_i^{(c)} c_{i\sigma}^{+} c_{i\sigma} + \sum_{i,j,\sigma} t_{ij}^{(d)} d_{i\sigma}^{+} d_{j\sigma}$$

$$+ \sum_{i,\sigma}{}' V_i^{(d)} d_{i\sigma}^{+} d_{i\sigma} + V \sum_{i,\sigma} (c_{i\sigma}^{+} d_{i\sigma} + d_{i\sigma}^{+} c_{i\sigma}) - \sum_i G_i \, (g_i - 1) \, \boldsymbol{S}_i \cdot \boldsymbol{s}_i$$

$$(-1/2)\mu_{\mathrm{B}} h \sum_i g_i^{(c)} (n_{i\uparrow}^{(c)} - n_{i\downarrow}^{(c)}) - \mu_{\mathrm{B}} h \sum_{i,\sigma} (g_i - 1) S_i^z . \qquad (1)$$

The notation in Eq. (1) is standard. The $c_{i\sigma}^{+}(d_{i\sigma}^{+})$ represent the creation operators for the electrons at Wannier states $\boldsymbol{R}_i$ for two different bands, $V_i^{(c)}, V_i^{(d)}$ stand for the positions of their centers of gravity, V is the parameter responsible for the on-site hybridization, G_i is the exchange integral between the spin operator $\boldsymbol{S}_i$ formed by the $4f$ RE electrons and $\boldsymbol{s}_i$ describes the spin density operator of the $c_{i\sigma}^{+}$-type electrons. All $G_i, V_i^{(c)}, V_i^{(d)}$ are of stochastic character dependent on a kind of the RE atoms which occupy the site $\boldsymbol{R}_i$ of the alloy realization.

The approximations are needed in order to handle the main physical properties of the Hamiltonian (1). We are interested in the dc resistivity and the thermo-electric power (TEP) contributions caused by the exchange interaction between localized $4f$ electrons (represented here by $\boldsymbol{S}_i$) and the itinerant $c_{i\sigma}^{+}$ electrons at high temperatures. Approximately those contributions to the total resistivity or TEP can be separated from the experimental results.

By the high temperature T we mean the temperature greater than the magnetic Curie temperature and high enough in order to thermally populate all one-particle states produced by the exchange interaction $-(g_i - 1)\boldsymbol{S}_i \cdot \boldsymbol{s}_i$. The exchange interaction produces two degenerated multiplets with the single site energies $+G(g_i - 1)S$ and $-G(g_i - 1)(S + 1)$. The degeneracy of the levels is S and $S + 1$, respectively. For such simplified system (the Hamiltonian has one electron stochastic form) the coherent potential formalism (CPA) [4–7, 9, 10] was applied. The electronic structure and the nature of quasiparticles for the similar system were discussed also in [9, 10, 11, 13]. In order to have the reference results we switched off the external field h and considered the system with the one-band (of the $c_{i\sigma}^{+}$-type) only. In order to calculate the electrical resistivity and TEP within the CPA approach it is important to know the changes of the DOS structure (the shape and positions of the peaks) around the E_{F} upon alloying. Figure 1 presents the summed s, p, and d DOS of Gd_2In and $(Gd_{0.5}Y_{0.5})_2In$. An analysis of Fig. 1 shows that the replacement of Gd with isoelectronic Y atoms removes the sharp peak of d-DOS from below the E_{F}, broadens and shifts the d-states DOS around the E_{F} to higher energies. From the results presented in Fig. 2a it is possible to recognize the mechanism of the electron scattering. For a

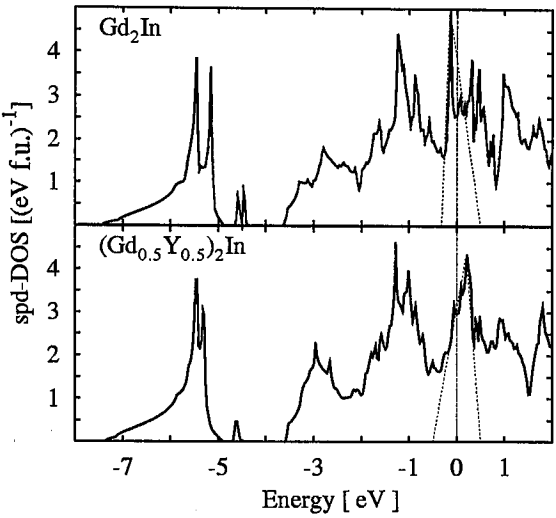

Fig. 1. Total *spd*-DOS for Gd_2In and $(Gd_{0.5}Y_{0.5})_2In$. Dot triangles represent approximate DOS used in the resistivity calculations. The dash vertical line crossing both parts of the figure depicts the Fermi energy.

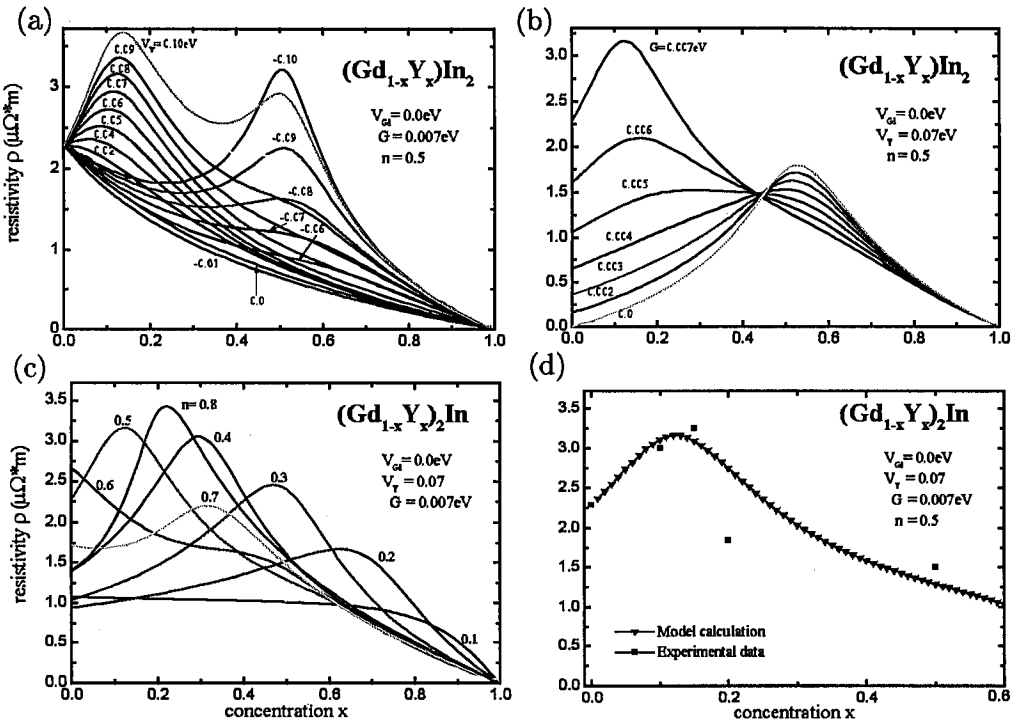

Fig. 2. The results of the high temperature spin disorder resistivity calculations for different sets of the model parameters.

high concentration of the Gd atoms ($x \ll 1$) the scattering on the different atomic levels is rather weak. For a higher concentration ($x \simeq 1$) the electrons scattering on Gd spins become less important and the resistivity part due to the scattering on different atomic levels increases. There is a concentration for which the resistivity reaches maximum. Simultaneously with a decreasing number of Gd atoms the system becomes uniform again and the effect of the atomic scattering becomes less important. In Fig. 2b the resistivity versus concentration x for several values of the $s-f$ interaction constants G was plotted. The resistivity increases and shows a maximum for lower concentrations. The maximum of the resistivity in the concentration range from 0 up to 0.15–0.20 causes the strong enough exchange interaction. Figure 2c shows how the resistivity depends on the average number n of the electrons in the band. The calculations within the presented model and the experimental resistivity results [14], as a function of the concentration x, are plotted in Fig. 2d. The results are very sensitive to the choice of the starting density of states of the pure systems. The TEP and the magnetoresistance for the systems described by Kasuya [1] are under consideration.

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