9.7 cm

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

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The electronic structure of the ferromagnetic Gd_2In and $(Gd_{1-x}Y_x)_2In$ compounds has been calculated with the use of self-consistent TB-LMTO method. Based on the potential parameters obtained the XPS spectra were calculated and compared with the experimental results. Calculations have shown that the density of states near the Fermi energy is dominated by $5d$-states of Gd, what can indicate that the indirect coupling of the Gd $4f$–magnetic moments is mediated by the strongly correlated $5d$ band.
The magnetic part of the electrical conductivity as a function of temperature in the considered alloy systems was analyzed. For the conductivity we have used the formula $\sigma^{xx} = \frac{\hbar e}{6\Omega_a}\sum_\sigma v^2/Im\Sigma_\sigma(\mu)$, where the $\Sigma_\sigma(\mu)$ describes the self energy of the electronic system which undergoes the scattering, the other quantities in the formula describe the system. The main interaction which causes the finite magnetic part of the conductivity was taken as a usual stochastically distributed in space $s-f$ type form. The band structure calculations which were performed give the necessary information on the number of scattering initial,final states $|\mathbf{k},spd,\sigma >$. Influence of the temperature in the range $[0, T_C]$ was discussed. The preliminary results for conductivity of $(Gd_{1-x}Y_x)_2In$ alloys qualitatively reproduce the experimental data.

13.4 cm

Subject category :

4. Rare Earths and Actinides, Alloys and Compounds

Presentation mode :
poster

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