MAGNETIC AND ELECTRONIC PROPERTIES OF DISORDERED $(Gd_{1-x}Y_x)_7Pd_3$ ALLOYS – THEORETICAL STUDY

A. Woźniakowski[a], W. Borgieł[b], J. Deniszczyk[a]

[a]Institute of Materials Science, University of Silesia, 40-007 Katowice, Poland
[b]August Chełkowski Institute of Physics, University of Silesia, 40-007 Katowice, Poland

9.7 cm

Recently the $(Gd_{1-x}Y_x)_7Pd_3$ alloys were the subject of intensive experimental investigations due to their potential magnetocaloric applications. The Curie temperature of Gd_7Pd_3 compound is too high for magnetocaloric applications but it can be tuned to appropriate value by partial substitution of Gd atoms by non-magnetic Y ones. In the entire concentration range the $(Gd_{1-x}Y_x)_7Pd_3$ alloys crystallize in the Th_7Fe_3 structure. In the paper we present the theoretical investigations of the electronic and magnetic structure and properties of $(Gd_{1-x}Y_x)_7Pd_3$ alloys. For the purpose of the electronic structure calculations the alloying was simulated within the supercell approach, with different local atomic configurations taken into account. The *ab-initio* calculations were performed applying the FP-LAPW method with the GGA-LSDA exchange-correlation potential. For the $4f$ states of Gd the enhanced Coulomb correlation term was included. Basing on the results of *ab-initio* calculations the many particle generalized s-f model for disordered alloy with strongly correlated band electrons was parametrized. With the use of Coherent Potential Approximation formalism the concentration dependence of Curie temperature and electrical conductivity in the paramagnetic state was determined. The results of calculations concide quantitatively with available experimental data.
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Corresponding author :
Władysław Borgieł

Address for correspondence :
August Chełkowski Institute of Physics, University of Silesia
Uniwersytecka 4, 40-007 Katowice, POLAND

Email address :
wladyslaw.borgiel@us.edu.pl