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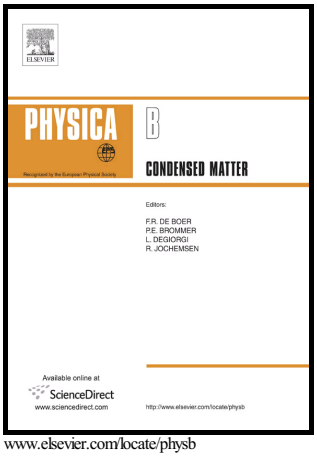


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# Electronic structure of $RSn_{1.1}Ge_{0.9}$ (R = Dy, Ho) ternary compounds: band calculation and optical properties

Yu. V. Knyazev[a], A. V. Lukoyanov[a,b], Yu. I. Kuz'min[a], S. Gupta[c], K.G. Suresh[c]

[a] *Institute of Metal Physics UD of RAS, Ekaterinburg 620137, Russia;*

[b] *Ural Federal University, Ekaterinburg 620002, Russia;*

[c] *Department of Physics, Indian Institute of Technology Bombay, 400076 Mumbay, India*

Abstract

The results of investigations of the electronic structure and optical properties of the compounds $DySn_{1.1}Ge_{0.9}$ and $HoSn_{1.1}Ge_{0.9}$ are presented. Our spin-polarized calculations of the electronic structure are carried out in the local spin density approximation with correction for strong electronic correlations (LSDA+*U* method) in the 4f shell of the rare-earth ion. In the wavelength range 0.22 – 15 μm, the optical constants of the intermetallic compounds were measured by the ellipsometric method, and a number of spectral and electronic characteristics are determined. Based on the calculated densities of states, the structural features of the optical conductivity in the region of interband light absorption are interpreted.

Keywords:

rare earth alloys and compounds; electronic band structure; optical properties, optical spectroscopy



## 1. Introduction

Interest in study of ternary intermetallic compounds the family RTX (where R and T are rare-earth and p- or d-metal respectively, X – p-element), in particular, is stimulated by the prospects of obtaining new materials with functionally prominent properties. In recent years, similar intermetallic compounds have been obtained in various compositions, including ones with magnetic or non-magnetic transition metals. Their physical parameters, as well as the types of crystalline and magnetic structures, vary considerably depending on the constituent elements. Along with a wide variety of electronic and magnetic properties, these compounds have a number of technically attractive characteristics, for example, giant magnetocaloric and magnetoresistance effects, which allow them to be considered as promising materials for practical use, see review [1] for further references. Such compounds include a series of intermetallics of almost equiatomic composition $RSn_{1.1}Ge_{0.9}$ (R = Dy, Ho) with orthorhombic