THE SUMMARY OF Ph. D. DISSERTATION

Major Fundamental Science and Technology SURNAME, Firstname

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Title

Magnetoelastic effects in rare-earth compounds RVO₄ and RPO₄

Abstract

The wave functions of the rare-earth ions in RVO_4 and RPO_4 are mainly determined by the crystal-field imposed on the 4*f* electrons. The variation of the crystal-field caused by strains corresponds to the one ion magnetoelastic coupling which describes the coupling between 4*f* electronic states and deformations of the lattice. This coupling leads to various characteristic features of the crystalline lattice.

X-ray diffraction measurements performed on $ErVO_4$ and $ErPO_4$ revealed anisotropic thermal expansion. It has been known that, in the cases of many RVO_4 and RPO_4 , the anisotropic thermal expansion can be explained in terms of the quadrupolar interaction of the 4*f* electronic states with the lattice. In contrast, the contribution from the sixth-order interaction was found to be essential in order to explain the thermal-expansion anomalies found in $ErVO_4$ and $ErPO_4$. From detailed analysis of the crystal-field, it was concluded that the sixth-order term of the crystal-field Hamiltonian has a major effect on energy levels of Er ions.

As a result of the magnetoelastic coupling, a cooperative Jahn-Teller phase transition involving a distortion of B_{2g} symmetry occurs in TbVO₄. The Jahn-Teller transition of the same type does not occur in TbPO₄. The Jahn-Teller transitions were observed for mixed crystals TbV_{1-x}P_xO₄ $(0 \le x \le 0.32)$ by X-ray diffraction techniques. A striking reduction in the transition temperature with increasing P concentration was observed. This reduction is a result of lowering of the local symmetry of the crystal-field due to random distributions of V and P atoms. The results of the diffuse scattering measurements performed on the x = 0.32 crystal indicated the existence of local strains.

The present analysis of the observed magnetoelastic effects should shed light on the fundamental mechanism of orbital ordering in d- and f- electron compounds.