EPJ Web of Conferences **132**, 03004 (2017) DOI: 10.1051/epjconf/201713203004
SPECTROSCOPY.SU 2016

Deformation splittings in the spectra of $LaAlO_3$: Ho^{3+}, Pr^{3+}, Tm^{3+} single crystals

K.N. Boldyrev[1,*], P. Dereń[2], and M.N. Popova[1]

[1]Institute for Spectroscopy RAS, 108840 Troitsk, Moscow, Russia
[2]Institute of Low Temperature and Structure Research, Polish Academy of Sciences, 50-950 Wroclaw, Poland

Abstract. The work is devoted to a high-resolution spectroscopy study of the perovskite-type single crystals of $LaAlO_3$ doped with non-Kramers rare-earth ions of praseodymium, holmium and thulium. Doublets of a specific shape were observed in the spectra, which we attribute to the presence of random deformations in the crystals.

It has been shown earlier that for dielectric crystals doped with rare-earth (RE) ions random deformations of the crystal lattice may result in a specific shape (with a narrow dip in the center) of spectral lines corresponding to transitions between crystal-field (CF) singlets (or Kramers doublets) and non-Kramers doublets [1-3]. In particular, a well resolved splitting of RE spectral lines caused by random lattice strains was observed in the spectra of tetragonal centers in $LiYF_4$:Tm^{3+} [1] and $CaWO_4$:Ho^{3+} [3] crystals and of cubic centers in hexafluoroelpasolite crystals doped with Sm, Er, Tm, or Yb [2]. It is of interest to observe such effect in the spectra of trigonal centers, in which non-Kramers ions also possess doubly degenerate CF levels.

We have chosen a $LaAlO_3$ crystal that belongs to the family of perovskites, possesses a pseudo cubic structure, and has a promising application potential. RE^{3+} ions in this compound substitute for La^{3+} which occupies a single crystallographic position with the D_3 point symmetry. There are Γ_1 and Γ_2 singlet and Γ_3 doublet CF levels for a non Kramers RE^{3+} ion residing in the D_3 symmetry position. Optical properties of $LaAlO_3$ doped with Pr^{3+}, Ho^{3+}, and Tm^{3+} ions were studied in Refs. [4-7] under a medium spectral resolution. In this work, we have measured high-resolution (0.02 cm^{-1}) broad-band (2000-20000 cm^{-1}) temperature-dependent transmission spectra of $LaAlO_3$ single crystals doped with non Kramers RE ions Ho^{3+}, Pr^{3+}, or Tm^{3+}. A splitting of several spectral lines corresponding to the Γ_1, $\Gamma_2 \rightarrow \Gamma_3$ transitions was observed (see, e.g., Fig. 1). We attribute this splitting to a combined action of the magnetic hyperfine interaction and random deformations of the crystal lattice.

The theory developed in Refs. [1-3] enabled to successfully model the line shapes and gave a tool for getting a quantitative estimate for the concentration of intrinsic lattice defects, by comparing experimental and calculated spectral shapes. To perform such calculations, the CF and electron-deformation interaction parameters are necessary. These

* Corresponding author: kn.boldyrev@gmail.com

parameters can be obtained from the CF calculations based on the experimentally found scheme of the CF levels and from the data of piezospectroscopic measurements. In this work, by analyzing high-resolution temperature-dependent transmission spectra of $LaAlO_3:Pr^{3+}$(0.1 at. %) single crystals we have determined energies of the CF levels of Pr^{3+} in the energy range up to 20000 cm^{-1}.

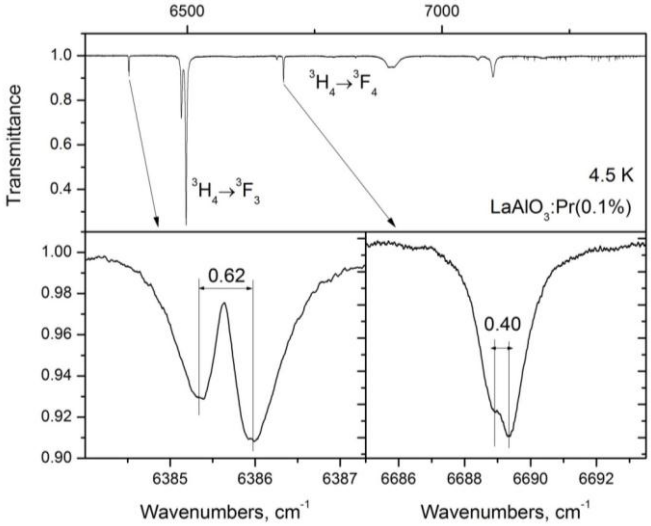

Fig. 1. A part of the Pr^{3+} spectrum in a $LaAlO_3:Pr^{3+}$(0.1 at. %) single crystal at the temperature 4.5 K. The lower part of the figure shows a doublet structure of some lines.

This dataset forms a basis for the CF calculations, a further modeling of deformation splittings observed in the spectra of trigonal RE centers, and, in this way, for development of a method to estimate the quality of perovskite crystals, which are known for a vast variety of applications.

References

1. S.A. Klimin, D.S. Pytalev, M.N. Popova, B.Z. Malkin, M.V. Vanyunin, S.L. Korableva, Phys. Rev. B **81**, 045113 (2010)
2. B.Z. Malkin, D.S. Pytalev, M.N. Popova, E.I. Baibekov, M.L. Falin, K.I. Gerasimov, N.M. Khaidukov, Phys. Rev. B **86**, 124406 (2012)
3. G.S. Shakurov, E.P. Chukalina, M.N. Popova, B.Z. Malkin, A.M. Tkachuk. Phys. Chem. Chem. Phys. **16**, 24727 (2014)
4. P. Dereń, J. Lumin. **122–123**, 40 (2007)
5. M. Malinowski, M. Kaczkan, S. Turczyński, D. Pawlak, Opt. Mater. **33**, 1004 (2011)
6. P. Dereń, J.-C. Krupa, J. Alloys Comp. **380**, 362 (2004)
7. A. Gocalińska, P. Dereń, P. Głuchowski et.al., Opt. Mater. **30**, 680 (2008)