CHARACTERIZATION OF $LuVO_4$:Yb SINGLE CRYSTALS

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Rare earth orthovanadates (RVO_4) have been reported to be applicable, in particular, as laser materials (see *e.g.* Ref. [1]), for remote thermometry, as catalysts *etc*. One of recently studied orthovanadates is $LuVO_4$, due to its optical properties (applicable in laser-diodes [2], optical waveguides [3]). These materials typically crystallize in zircon-type structure. For applications as a single crystal, the defect structure of such crystals has to be studied. Obtaining of defect and electron structure is important for modelling of material properties. Up to now, defect structure of RVO_4 single crystals has not been widely studied. $LuVO_4$:Nd and a $GdVO_4$ single crystals of >2 cm size were grown by Czochralski method [3,4], providing 200 rocking curve FWHM of 67 arcsec width; the observed defects included cracks, inclusions (due, in particular, to the interaction with Ir crucible), large voids, and dislocations. Czochralski-grown YVO_4 crystals of >5 cm size exhibit dislocations, glide bands, subgrain boundaries with misorientations of several up to 40 arcmin [5,6].

The needle-shaped (up to $1\times2\times12$ mm^3 size) crystals of $LuVO_4$ were grown from PbO/PbF_2 flux by the slow cooling method. Defect properties of $LuVO_4$:Yb were studied using x-ray topography and high resolution (HR) diffraction, electronic structure of crystal has been analyzed by x-ray photoelectron spectroscopy (XPS) method.

The examined $LuVO_4$:Yb crystal was built from two parts, a lighter (transparent) part and a darker part. The HR diffraction study was performed using the PHILIPS-MRD diffractometer equipped with Cu tube (λ = 1.54056 Å), a four bounce Ge(022) monochromator and a two bounce Ge(022) analyzer. The XPS spectra were recorded in the Perkin-Elmer 5400 ESCA spectrometer, with use of Mg Kα (1253.6 eV) excitation mode. Projection reflection topographs were recorded at the F1 beamline (DORIS III, Hasylab).

The HR diffraction curves were obtained for the 002 reflection. The results show that two parts of crystal differed by defect structure: the light part is a true single crystal, whereas the dark part is built from several slightly misoriented blocks. The lattice parameter for light and dark parts is the same $a_\perp$ = 7.0244(2) Å. The reflection topographs reveal the defect structure in the vicinity of the (100) oriented crystal surface. A small part of the studied crystal is misoriented by several degrees. The kind of the contrast observed shows that the defects (dislocations or inclusions) are homogeneously distributed along the crystals.

The analysis of the acquired XPS spectra of $LuVO_4$:Yb showed that the shape of the V 2*p* spectrum closely resembles the relevant one of a V_2O_5 oxide. No line of the dopant could be detected. This also refers to a full consistency of their bond energies (of V $2p_{3/2}$ line) and spin-orbit splitting, Δ. Therefore, the bond energies of V 2*p* core-levels in $LuVO_4$ remain influenced only by oxygen ligand. The Lu 4*f* XPS spectrum absolutely dominates the valence band region built of O 2*p* states. Its shape exhibits close similarity to that of pure Lu. With the same value of spin-orbit splitting, its bond energy of $4f_{7/2}$ peak remains only shifted by 0.5 eV to higher values as a result of binding with oxygen ligand. This indicates strongly localized character of the Lu 4*f* level within the valence band.

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