Zr-Containing Oxide Compounds: Structure and Optical Properties

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Zirconium-containing oxide compounds have been actively studied as perspective materials for various applications: mercury-free lamps, luminescent probes, luminescent materials for solid state lighting, catalyst support, sodium or lithium ion batteries etc. Variety of structures ranging from relatively simple ZrO2 to complex langbeinite-type KZr2(PO4)3 and K2BiZr(PO4)3 crystals provides good opportunity to study structure-properties relationships, in particular role of ZrO2 polyhedra in luminescence processes. The most of Zr-containing oxides compounds are insulators with typical band gap values ~ 5 eV [1-3] but these compounds often show an intensive host-related photoluminescence (PL) in the visible spectral region. Obviously, mentioned luminescence is associated with defect-related luminescence centers. The doping with various ions is the most common way to affect the number of defects and therefore to improve optical properties of these oxide compounds.

In this work the structure and luminescence properties of the set of Zr-containing oxide compounds were studied by means of XRD, SEM and luminescence spectroscopy and by electronic band structure calculations. The VUV-excited luminescence properties were measured in 3.5–20 eV region of excitations energies in the 10 - 300 K temperature range. Dependencies of the PL intensities on temperature were obtained for different excitation wavelengths. Luminescence spectra for excitation with N2-laser (λex = 337.1 nm) and three diode-pumped (λex = 405, 473 and 532 nm) radiation also were obtained. The electronic structure calculations for ideal and defect-containing crystals were performed by full-potential linear-augmented-plane-wave method implemented in the Wien2K package [4].

The results of experimental the PL studies are discussed together with electronic band structure calculations results, and literature data. The impact of fluorination on the host-related and RE-related luminescence was studied for the case of ZrO2 compounds. Influence of the rare-earth doping on the ZrO2, KZr2(PO4)3 and K2BiZr(PO4)3 compounds are discussed too.