Experimental and Numerical Investigation of Photoluminescence in Rare-earth Doped $LiBa_{12}(BO_3)_7F_4$ (LBBF) crystals

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The study of borate systems is a research field developing strongly at the intersection of crystal chemistry and material science. Borates are very promising compounds due to their chemical diversity and many areas of practical application [1-3].
The compound $LiBa_{12}(BO_3)_7F_4$ (LBBF) was first described by Zhao and Li [4] and its structure was reinvestigated in Ref. 5. The LBBF crystal belongs to the group of "antizeolite" borates with a $[Ba_{12}(BO_3)_6]^{6+}$ cation "framework" (ideal symmetry *I*4/*mcm*) and (pseudo)tetragonal channels along *c* axis formed by altering cubes and anticubes of barium atoms. Cubic cages are occupied by $[LiF_4]^{3-}$ clusters, whereas anti-cubes are occupied by $(BO_3)^{3-}$ groups. Thus, the structural formula of LBBF can be represented as $Ba_{12}(BO_3)_6[BO_3][LiF_4]$.
Luminescent properties of LBBF doped with Eu^{3+}, Tb^{3+}, Ce^{3+} in different combinations were recently studied [6]. It was assumed that the multiband photoluminescence of LBBF:Eu^{3+}, Tb^{3+}, Ce^{3+} crystals allows obtaining white-color luminescence by selecting the optimal concentration ratio of rare-earth elements and the optimal excitation wavelength. Single crystals of undoped and Ce^{3+}, Tb^{3+}, and Eu^{3+}/Tb^{3+}/Ce^{3+} co-doped LBBF crystals were grown from high-temperature solutions. The shape and position of lines in the photoluminescence spectra in the range of 77-300 K were typical of cerium, terbium, and europium ions. Luminescence lifetime constants were measured in the range of 77-300 K. No processes of energy transfer were defined. It was shown that at the excitation wavelength of 370 nm at 300 K, LBBF:Eu^{3+}, Tb^{3+}, Ce^{3+} crystals have luminescence close to daylight with CIE chromaticity coordinates and correlated color temperature of (0.295; 0.362) and 7121 K, respectively.
A combined experiment plus computation effort allows to identify and interpret electronic and optical properties of LBBF:Ce^{3+} crystals [7].
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