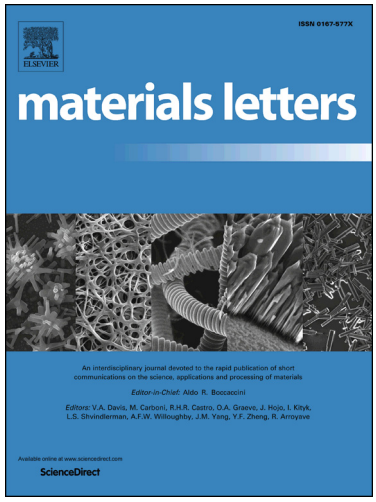

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Acceptor doping, hydration and band-gap engineering of $BaZrO_3$

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Abstract

Yttrium-doped $BaZrO_3$ powders have been synthesized by sol-gel method. Powder XRD confirms that $BaZr_{1-x}Y_xO_{3-\delta}$ (x=0.00, 0.05, 0.10) crystallize with the perovskite-type unit cell (space group $Pm\bar{3}m$). The effect of doping and hydration on the band gap of $BaZr_{1-x}Y_xO_{3-\delta}$ has been revealed from the analysis of the diffuse reflection spectra. An additional absorption band is observed near the fundamental absorption edge in the doped samples annealed in dry oxygen. The found effect is explained by the impact of defects on O(2*p*)–Zr(4*d*) charge transfer transitions and the trapping of electrons by oxygen vacancies.

Keywords

Crystal structure
Defects
Optical materials and properties
Spectroscopy

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