Surface morphology and control of optical band gap in blue-green-orange-red photoluminescence of $Ba[Zr_{0.25}Ti_{0.75}]O_3$ thin films

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Recently, the barium zirconate titanate, $Ba[Zr,Ti]O_3$ (BZT), has been chosen as an alternative material to barium strontium titanate, $[Ba,Sr]TiO_3$ (BST), in the preparation of thin films or ceramic bulks This material presents a perovskite-type structure with general formula ABO_3 (A site = Ba and B site = Ti,Zr). Generally, BZT are formed by solid solution between barium titanate (BTO) and barium zirconate (BZO) due to the substitution of the Ti^{4+} ions (B site) (atomic weight of 47.9, ionic radius of 74.5 pm) by Zr^{4+} ion (atomic weight of 91.2, atomic radius of 86 pm). This substitution is possibly due to the Zr^{4+} ions to be chemically more stable than the Ti^{4+} ions [1–3].

Blue-green-orange-red photoluminescence (PL) emission at room temperature was observed in $Ba[Zr_{0.25}Ti_{0.75}]O_3$ (BZT) thin films prepared by the complex polymerization method and heat treated at 400°C for different times. PL emission was not verified for the BZT thin films heat treated at 700°C for 2 h in air atmosphere. BZT thin films were characterized by X-ray diffraction (XRD), Fourier-transform infrared (FT-IR) spectroscopy and Ultraviolet-visible (UV-vis) absorption spectroscopy.

XRD patterns showed that BZT thin films are free of deleterious phases and crystallize in a cubic structure. FT-IR measurements suggest that the increase of heat treatment temperature and processing time promote an increase of the $[Zr,TiO_6]$ stretching mode. UV-vis measurements indicated the presence of localized states into the band gap of disordered BZT thin films heat treated at 400°C for different times. The morphology and thickness of BZT thin films were investigated by field emission gun-scanning electron microscopy (FEG-SEM) and atomic force microscopy (AFM). FEG-SEM and AFM micrographs revealed that the surface morphology and thickness of BZT thin films are influenced by the heat treatment time. BZT thin films with structural order-disorder exhibited a blue-green-orange-red photoluminescence emission at room temperature, which can be related with the presence of localized states (shallow and deep holes) into the band gap.

Keywords: Surface morphology; Optical band gap; Photoluminescence and BZT thin films.

Work supported by CAPES, FAPESP – CEPID and CNPq.

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