

Effect of Barium Doping on Structural, Morphological, Optical, and Photocatalytic Properties of Sprayed ZnO Thin Films

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Abstract : Thin films of pure and barium-doped zinc oxide (ZnO) were prepared using spray pyrolysis process. The films were deposited on glass substrates at 450°C. The different samples are characterized by X-ray diffraction (XRD) and UV-Vis spectroscopy. X-ray diffraction patterns reveal the formation of a single ZnO Wurtzite structure and the good crystallinity of the films. The substitution of Ba ions influences the texture of the layers and makes the (002) plane a preferential growth plane. At concentrations below 6% Ba, the hexagonal structure of ZnO undergoes compressive stresses due to barium ions which have a radius twice of the Zn ions. This result leads to the decrees of a and c parameters and therefore the volume of the unit cell. This result is confirmed by the decrease in the number of crystallites and the increase in the size of the crystallites. At concentrations above 6%, barium substitutes the zinc atom and modifies the structural parameters of the thin layers. The bandgap of ZnO films decreased with increasing doping, this decrease is probably due to the 4d orbitals of the Ba atom due to the sp-d spin-exchange interactions between the band electrons and the localized d-electrons of the substituted Ba ion. Although, the Urbache energy undergoes an increase which implies the creation of energy levels below the conduction band and decreases the band gap width. The photocatalytic activity of ZnO doped 9% Ba was evaluated by the photodegradation of methylene blue under UV irradiation.

Keywords : barium, doping, photodegradation, spray pyrolysis, ZnO.

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