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Experimental and theoretical analyses of the nonlinear optical effects in Magnesium and Copper co-doped Zinc Oxide nanorods

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Abstract

Magnesium and Copper co-doped Zinc oxide nanorods (ZnO NRs) were grown on glass substrates applying hydrothermal technique. They were investigated with respect to their structural and morphological insights through X-ray diffraction (XRD) patterns, field emission scanning electron microscope (FESEM) and atomic force microscope (AFM) technique. The nanorod diameters were found to vary within 105 nm – 153 nm. The nanorods were hexagonal in shape with wurtzite structure and oriented along *c*-axis. Band gap magnitudes were evaluated from the UV-Visible absorption spectra and were found to be higher for Mg5%Cu2%ZnO nanorod sample owing to its smaller crystallite size. Photo-polarization did the additional alignment in the nanorod samples to observe optical nonlinearity of the first and second order. When the spectral energy of the laser beam matched with the energy of the absorption band edge of the samples, we observed also third harmonic generation (THG) besides second harmonic generation (SHG). Quantum chemical calculation using norm-conserving pseudo-potential method was applied to confirm the origin of the effects.

Keywords: ZnO nanorods; hydrothermal technique; photo induction; second harmonic generation; third harmonic generation;

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