Structural and Optical Modulation of ZnO Thin Films via Fe Doping

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ABSTRACT

In this study, ZnO and Fe-doped ZnO thin films were synthesized via the sol-gel spin coating technique to investigate the influence of iron doping on their structural, morphological, and optical properties. Zinc acetate dihydrate was used as the Zn source and iron nitrate as the dopant. Monoethanolamine (MEA) served as the stabilizer while 2-methoxyethanol was employed as the solvent. Additionally, polyvinylpyrrolidone (PVP) was added to enhance the surface quality of the films. Fe was introduced at 0.1 M, 0.2 M, and 0.3 M concentrations relative to Zn. The average film thicknesses were measured to be between 45 and 65 nm.

X-ray diffraction (XRD) analyses confirmed the formation of hexagonal wurtzite structure in all samples, with no indication of secondary phases such as Fe oxide, suggesting successful incorporation of Fe ions into the ZnO lattice. Increasing Fe content resulted in a decrease in crystallite size from 24.1 nm (pure ZnO) to 16.5–17.0 nm, indicating grain refinement due to Fe substitution. Furthermore, microstrain (ε) and dislocation density (δ) values increased significantly, reflecting increased lattice disorder.

SEM and Gwyddion-assisted 3D surface analyses revealed a clear evolution in surface morphology. Pure ZnO exhibited a granular and rough surface, while Fe-doped samples, especially at 0.3 M, displayed smoother, denser, and more uniform surfaces. Surface roughness decreased dramatically, indicating improved film quality with increasing Fe concentration.

Optical characterization via UV-Vis spectroscopy showed a reduction in absorbance and a red shift in absorption edge as Fe content increased. Tauc plots revealed that the optical band gap increased from 3.39 eV for pure ZnO to 3.90, 3.93, and 3.95 eV for 0.1 M, 0.2 M, and 0.3 M Fe-doped ZnO, respectively.

In summary, Fe doping notably modifies the structural compactness, defect density, band gap energy, and surface quality of ZnO films, rendering them promising for applications in optoelectronics, photodetectors, and solar energy devices.

Keywords— *ZnO thin films, Fe doping, sol-gel method, XRD, SEM, UV-Vis, band gap*