Evolution of structural phase transition from hexagonal wurtzite ZnO to cubic rocksalt NiO in Ni doped ZnO thin films and their electronic structures

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Abstract

This study thoroughly examines the collective influence of compositional variation and annealing temperature on the electronic structure of sol-gel derived NixZn1-xO (x = 0 to 1) thin films annealed at different temperatures (700°C, 800°C, and 900°C) using X-ray photoelectron spectroscopy (XPS) and X-ray absorption spectroscopy. A gradual structural phase transition from hexagonal wurtzite ZnO to cubic rocksalt NiO with increasing Ni concentration was revealed by X-ray diffraction (XRD). Grain growth was observed from scanning electron microscopy with increasing annealing temperature. Photoluminescence measurements indicate the presence of defects like interstitial oxygen with Ni atoms incorporation. The Ni L3,2 absorption edge shows an intensity enhancement in the white-line feature with increasing Ni concentration, evidencing the presence of higher oxidation states. Concurring results were observed by XPS where both Ni2+ and Ni3+ free ion multiplets are present in Ni 2p core level spectrum for 20% and higher Ni concentration. O K and Zn L3,2 XAS spectra demonstrated the eg-t2g sub-band splitting at higher Ni concentration, triggered by band anticrossing interaction and crystal field splitting. The extended X-ray absorption fine structure (EXAFS) simulation for the Zn K edge revealed a Zn-Zn/Ni bond length change for 60% Ni concentration. The thermal disorder factor increased up to 40% Ni concentration, and beyond that, it decreased due to stable NiO phase dominance in the alloy composite. Ni K edge EXAFS fitting indicated an insignificant change in the Ni-O and Ni-Ni/Zn bond lengths throughout the range of varying Ni concentrations. The thermal disorder factor increases with increasing annealing temperature, indicating a more disordered lattice. Such investigation has importance where the performance of functional devices is determined by the electronic properties of nanometer sized materials. In a nutshell, the present work critically elucidates the combined impact of compositional variations and annealing temperatures on electronic structures.