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Structural characterization of Zr-doped ZnO films deposited on quartz substrates by reactive radio frequency magnetron co-sputtering

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Abstract

Zr-doped ZnO ($Zn_{1-x}Zr_xO$, $0 \leq x \leq 0.067$; ZZO) thin films were grown at room temperature by reactive radio frequency co-sputtering on quartz substrates The ZZO films have a strong preferred orientation toward the c-axis but this orientation weakened as *x* increased. The size of crystallites of the ZZO films decreased and the surfaces of the ZZO films smoothened as *x* increased. The Zn atom were divalent and slightly affected only in the *c*-axis. Zn *K*-edge X-ray absorption near edge structure (XANES) spectra of the ZZO films show that the Zn atom were divalent and slightly affected only in the *c*-axis. The Zr atoms were tetravalent and their *K*-edge XANES spectra were slight different from that of ZrO_2. Polarization-dependent Zn *K*-edge extended x-ray absorption fine-structure (EXAFS) spectra revealed that the local structural variation was stronger along the *c*-axis than along other axes. The Zn atom site was well replaced by Zr atom regardless of *x*. Average optical transmittance in the visible region was ≥ 90%, and as *x* increased, optical band gap increased and blue-shifted.

Keywords: Transparent Conducting Oxide, X-ray Diffraction, X-ray Absorption Near Edge Spectroscopy, Extended X-ray Absorption Fine Structure, Energy Band Gap.
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