TT-P055

Energy Band Structure, Electronic and Optical properties of Transparent Conducting Nickel Oxide Thin Films on SiO_2/Si substrate

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Nickel Oxide (NiO) is a transition metal oxide of the rock salt structure that has a wide band gap of 3.5 eV. It has a variety of specialized applications due to its excellent chemical stability, optical, electrical and magnetic properties. In this study, we concentrated on the application of NiO thin film for transparent conducting oxide. The energy band structure, electronic and optical properties of Nickel Oxide (NiO) thin films grown on Si by using electron beam evaporation were investigated by X-Ray Photoelectron Spectroscopy (XPS), Reflection Electron Energy Loss Spectroscopy (REELS), and UV-Spectrometer. The band gap of NiO thin films determined by REELS spectra was 3.53 eV for the primary energies of 1.5 keV. The valence-band offset (VBO) of NiO thin films investigated by XPS was 3.88 eV and the conduction-band offset (CBO) was 1.59 eV. The UV-spectra analysis showed that the optical transmittance of the NiO thin film was 84% in the visible light region within an error of ±1% and the optical band gap for indirect band gap was 3.53 eV which is well agreement with estimated by REELS. The dielectric function was determined using the REELS spectra in conjunction with the Quantitative Analysis of Electron Energy Loss Spectra (QUEELS)-ε(κ,ω)-REELS software. The Energy Loss Function (ELF) appeared at 4.8, 8.2, 22.5, 38.6, and 67.0 eV. The results are in good agreement with the previous study [1]. The transmission coefficient of NiO thin films calculated by QUEELS-REELS was 85% in the visible region, we confirmed that the optical transmittance values obtained with UV-Spectrometer is the same as that of estimated from QUEELS-ε(κ,ω)-REELS within uncertainty. The inelastic mean free path (IMFP) estimated from QUEELS-ε(κ,ω)-REELS is consistent with the IMFP values determined by the Tanuma-Powell Penn (TPP2M) formula [2]. Our results showed that the IMFP of NiO thin films was increased with increasing primary energies. The quantitative analysis of REELS provides us with a straightforward way to determine the electronic and optical properties of transparent thin film materials.

Keywords: Energy band structure, Electronic properties, Optical properties, REELS, XPS, IMFP, NiO