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Title: Development of Metal oxide Nanostructured Thin Films for Sensor Applications

Research Findings

Over the past two decades, a lot of research endeavors have been directed toward the advancement of devices for sensing gas in practical applications ranging from toxic/inflammable gas detection to continuous environmental monitoring. The usage of gases has become increasingly important in both the domestic and industrial fields and owing to this reason it has become essential to fabricate extremely reliable gas sensors with the enhanced response. These sensors must support the uninterrupted supervision of certain gases existing in the surroundings in a selective and quantitative manner. Gas sensors based on semiconducting metal oxides have evoked a lot of interest and cover a wide range of applications. Currently, worldwide efforts are focused on both the basic as well as applied research areas, and there is continued interest in developing novel materials with innovative structures designed for enhanced response.

The content of the current thesis presenting the conducted research work has been split into five chapters as specified below:

Chapter 1, encompasses the introduction as well as the appraisal of the research work done up till now on thin films of metal oxide with specific attribution to the Nickle oxide, pure and doped ZnO. The investigation of the thin films of NiO and ZnO by different researchers has been deliberated. The inspiration, purpose, and possibility of the current work have been concisely defined.

Chapter 2, describes the aspects of experimental methods employed in the current research for the fabrication and characterization of thin films of Nickle Oxide and ZnO coated onto different substrates. To achieve thin films with single-phase and superior quality, they were annealed at varied temperatures under an oxygen atmosphere. The structural, electrical as well as optical investigations were accomplished for the thin films coated on substrates of glass and ITOcoated glass. The identification of phases, and lattice parameters, examine surface morphology and structure, microstructure, elemental analysis, absorbance or transmittance spectra, etc.

In Chapter 3, nanoparticles of nickel oxide (NiO) were prepared via wet chemical synthesis to be employed as a chemi-resistive chlorine (Cl_2) gas sensor in the 2-200 ppm range. The structural phase exhibited by the NiO nanoparticles in the sensing layer was cubic. The size of the NiO nanoparticles was determined to be 21 nm. The optical energy band gap was obtained to be 3.13 eV. At a moderate temperature of 200°C, Cl_2 gas with 10ppm concentration elicited a swift time for the response of 12 s and an optimum time for recovery of 27 s. These outcomes establish the potential of NiO nanoparticles for the synthesis of extremely selective and sensitive sensors for Cl_2 gas.

In chapter 4, ZnO thin films, with different concentrations of N, were fabricated using a spin coating device. The spectra obtained via X-ray diffraction (XRD) confirmed the (002) plane as the preferred orientation for the growth of all films. XRD and Raman's studies confirmed the single hexagonal phase of ZnO. The crystallite size was evaluated in the range of 25 to 36 nm. The elemental analysis by EDX verified the doping of N in ZnO and elemental mapping via SEM further verified its homogeneous distribution. The surface analysis by AFM ascertained the creation of spherical nanoparticles and also that the size of nanoparticles increased with an increase in N doping. The surface of all the films was well covered as observed in AFM images. The films were optically transparent, and the transparency was found at ~ 80%, which is pretty remarkable from the viewpoint of application to the window layer, however, it implies a very minute reduction due to N doping. The absorption edge was observed to shift towards longer wavelengths due to N doping, which indicates a drop in the energy gap. The energy gap was estimated by employing Tauc's equation and observed to decrease from 3.43 eV to 3.14 eV (ΔE = 0.29 eV). Index of absorption, refraction, and real as well as imaginary dielectric constants were also determined. The $\chi^{(1)}$ and $\chi^{(3)}$ values were evaluated to be in the range of 0.3 to 9 and 1.0 $\times 10^{-11}$ to 1.0 $\times 10^{-8}$, respectively. Thin films with spherical nano-crystallites, superior optical transmission, and nonlinear properties proposed their applications in optical sensors.

In Chapter 5, the outcomes and summary of the work along with a brief insight into the future potentials of the work have been discussed.