Abstract

Impact of Cu doping on the structure, morphology, optical properties, electrical resistivity, and antimicrobial activity of NiO thin films has been investigated for a broad range of Cu/Ni ratios (0.1 – 25%). These thin films were synthesized on pre-heated glass substrates using indigenous spray pyrolysis setup. The structural analysis via X-ray diffraction technique reveals that all the thin films are of polycrystalline nature with cubic structure. All the diffraction peaks shift towards lower angle on an increase in the Cu/Ni ratio. Texture coefficient and stacking fault probability were determined by Harris analysis and Warren–Warekois formula, respectively. Crystallite size and lattice strain were valued by means of Williamson–Hall analysis, size-strain plots, Scherer and Wilson formulae. The value of crystallite size shows a decreasing trend while lattice strain increases on increasing the Cu/Ni ratio. SEM micrographs of the thin films reveal that surface morphology consists of pores, and the density of these pores decreases as the Cu/Ni ratio increases. The characteristic absorption bands exhibited by FTIR spectra of un-doped NiO and NiO:Cu thin films recorded in the range 4000–450cm^{-1} were identified.

The optical analysis done via UV-Visible spectrophotometer reveals that absorption edge for all the films lies in the UV region and the average

reflectance of the films (λ = 280 – 900 nm) for all Cu concentration is 16.9 % with standard deviation of 1.38. Optical band gap of the thin films decreases while Urbach energy increases as Cu/Ni ratio is increased. The mean value of measured refractive index n (λ = 280 – 900 nm) increases with Cu/Ni ratio. As optical band gapincreases refractive index decreases. Quantitatively, mean value of measured refractive index is in good agreement with that derived from the Reddy-Ahammed empirical formula connecting optical band gap with refractive index. PL spectra exhibited strong peak at 403 nm shouldering with another peak at 426 nm, and one weak peak at 365 nm. For each peak in PL spectra, intensity is maximum in case of pure NiO thin film. As Cu concentration in NiO thin film increases from 0 to 3%, PL intensity decreases monotonically. With further increase in Cu content to 4%, intensity slightly increases and then remains almost independent of Cu/Ni ratio till 25 %. Both electrical resistivity and carrier mobility are found to decrease whereas carrier concentration increases with increase in Cu/Ni ratio.

Pure NiO thin film was found to be a poor antibacterial as well as antifungal agent against the *Escherichia coli* (*E. coli*), *Aspergillus niger* (*A. niger*) and *Macrophomina phaseolina* (*M. phaseolina*). However, its

antibacterial ability gradually increases on doping with 0.1 – 25 % Cu. Higher the Cu/Ni ratio, better is the antibacterial and antifungal response.

Ni_2O_3 thin films with seven molar concentrations ranging from 0.01 – 0.5 M were deposited on pre-heated glass substrates employing spray pyrolysis technique. Structure of the films was hexagonal with one major peak of (002) plane. Enhancement in crystallinity was observed on increase in molarity. Average optical absorbance in the visible region increases on increasing molarity. Both direct as well as indirect band gaps were found to decrease whereas Urbach energy increased on increasing molarity of the films. Optical reflectance was less than 10 %. In visible region, the average extinction coefficient increases while the average refractive index and the average optical reflectance decrease on increasing molarity. Surface morphology of the films consisted of random shape nanoparticles. Surface roughness of the films increased rapidly with molarity in the range 0.01 – 0.03 M, and then decreases to an intermediate level around which it undulated in the range 0.05 – 0.5 M.