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Structural and Optical Behaviour of Thermally Evaporated *p*-Type Nickel Oxide Thin Film for Solar Cell Applications

M.Vignesh Kumar[1], S. Muthulakshmi[1], A.Alfind Paulfrit[2],J.Pandiarajan[2], N.Jeyakumaran[2], N.Prithivikumaran[2]*

[1]Department of Physics, Sri VidyaCollege of Engg.&Tech., Virudhunagar –626 001, India.
[2]Department of Physics, VHNSN College (Autonomous), Virudhunagar – 626 001, India.

*Corres.author: janavi_p@yahoo.com

Abstract : Nickel oxide (NiO) thin films have been fabricated by thermal evaporation of nickel metal powder on glass substrate and oxidised through annealing to form nickel oxide thin films. The structural and optical properties of theNiO film annealed at 400^{o}C was examined by X-Ray diffraction (XRD), UV-Visible and Photoluminescence (PL) spectral studies. The XRD analysis of the prepared thin films reveals cubic structure with dominant (1 1 1) orientation. The grain size calculated by using Debye-Scherrer formula was 27 nm. From the XRD analysis the micro strain and the dislocation density was also calculated.The transmittance of the NiO films was 81% at 550nm wavelength. The direct and indirect band gaps derived from Tauc's plot are 3.61eV and 1.90eV respectively. The room temperature PL spectrum of the NiO thin film show a strong dominant peak at 495 nm along with shoulder peaks at 430nm and 390 nm with excitation at 290nm.These results show that NiO films could be a potential candidate for solar cell applications.
Keywords: NiO thin film, Thermal evaporation method, Structural and Optical properties.

Introduction

Nanostructured transparent conducting oxides(TCO) have been actively studied due to both scientific interest and potential applications.TCO films such as zinc oxide, tin oxide, indium tin oxide, cadmium oxide *etc.*, are in practical use for transparent electrodes and window coatings. All these films are *n*-type semiconductors. But *p*-type TCO thin films are required for applications like transparent electrodes for optoelectronic devices, which make use of hole injection. Nickel oxide (NiO) is an important antiferromagnetic *p*-type semiconductor with wide band gap of 3.15- 4.0eV[1]and cubic rock salt like crystal structure.It has an excellent chemical stability as well as optical, electrical and magnetic properties, which makes it an attractive material to have a wide application infuel cell, electrochromic devices, solar thermal absorber, lithium ion batteries, solar cells, antiferromagnetic layer,magnetic devicesand chemical sensor[2].Many researcher have fabricatedNiO films by various methods such as spray pyrolysis, chemical vapour deposition, electrochemical deposition, sputtering, sol-gel,thermal evaporation[3]*etc.*,Among the various methods, the thermal evaporation method yields greater uniformity on the substrate surface. In the present paper, we report the NiO thin films prepared by thermal evaporation method which is annealed at 400^{o}C. Their structural and optical properties are characterized by X-Ray diffraction (XRD), UV-Visible and Photoluminescence (PL) spectral studies.

Experimental Details

The films were deposited on non conducting microscopic glass substrate (2.5 cm x 2.5cm, 1.35 mm thickness). Initially before film deposition, the substrate was first kept in hot chromic acid bath at 90°C for 1 hour. Then the glass substrate was ultrasonically cleaned using ultrasonicator with distilled water for 30 minute and finally it was cleaned with acetone.Nickel films were deposited on the well cleaned glass substrate by evaporating high purity (99.9%) Nickel (Ni) powder from an electrically heated tungsten crucible at about 5 x 10^{-4} Pa(Joule effect). The distance between the substrate and the tungsten crucible is set as 7 cm. After deposition the film was annealed at 400°C for 1 hour. The obtained NiO film was subjected to XRD, UV–Visible and PL studies. The structural properties of the NiO films were examined using X'PERT PRO X-ray diffractometer which was operated at 40 KV and 30 mA. The Optical properties of the films were examined by SCHIMADZU 1800UV–Visible spectrophotometer in the range of 200-1100 nm wavelength.The PL spectra was recorded using OCEAN OPTICS JAZ Spectrophotometerat an excitation wavelength of 290 nm. All the measurements were carried out in room temperature.

Result and Discussion

Structural Properties – XRD analysis

The crystallinity, crystallite size, and crystal structure of the as-prepared NiO film was examined using by XRD method. The XRD pattern of the prepared NiO film annealed at 400°C was shown in Figure 1. It shows a dominant and a less intense peaks at 2θ = 37.28° and 43.23° which are assigned to (1 1 1) and (200) crystal planes respectively.

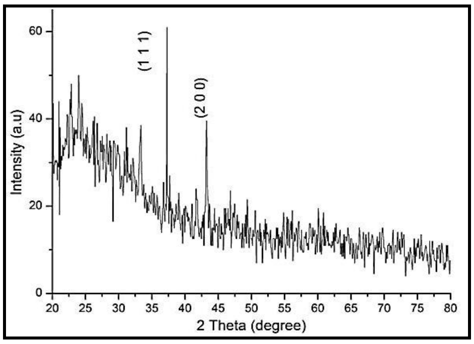

Figure1XRD pattern of NiO thin film annealed at 400°C

All these diffraction peaks can be perfectly indexed to FCC crystalline structure. Furthermore, no other peaks corresponding to other phases have emerged. The obtained XRD pattern is in excellent agreement with standard JCPDS (File No78-0643). Similar XRD pattern of cubic structure of NiO thin films can be observed in the literature reports[4,5]The crystallite size was calculated from the diffraction peak using the well-knownDebye – Scherrer formula,

$$D = \frac{k\lambda}{\beta \cos\theta} \quad .1$$

where D-crystallite size, k-0.94, λ-wavelength of X-ray, θ-angle of diffraction and β-Full Width at Half Maximum. The calculated crystallite size was 27 nm.The dislocation density (δ) which represents the amount of defects in the film was determined from the formula,

$$\delta = \frac{1}{D^2} \quad .\square.$$

whereδ is the dislocation density and D is the crystallite size.The estimated dislocation density was 0.137 x 10^{16} lines/m^2. The micro strain (μ) produced in the NiO thin films was calculated by using the formula,

$$\mu = \frac{\beta \cos\theta}{4} \quad .\square.$$

The calculated micro strain, grain size, dislocation density values are presented in Table 1. The occurrence of micro strain may be attributed to stretching and compression in the lattice. The lattice constant "*a*" for the cubic structure is given by the relation,

$$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2)}{a^2}$$

. □.

where "*d*" is the inter-planer distance and (*hkl*) are the Miller indices. The estimated lattice parameteris given in Table 1.

Table 1 Structural Parameters of 400°C annealed NiO Thin Film

Temperature	*D*(nm)	δ(x 10^{16} lines/m^2)	μ	*a* (Å)
400°C	27	0.137	0.0782	4.320

Optical Properties – UV Visible Analysis

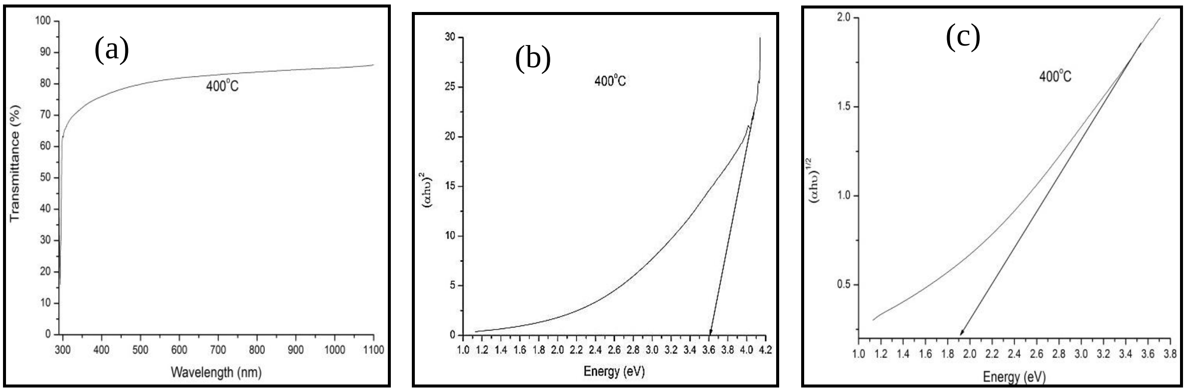

Figure 2 (a) Transmittance Spectra (b) Direct &(c) Indirect energy gap of NiO thin film

Figure 2(a) show the transmission spectra of the prepared NiO thin film annealed at 400°C. The transmittance of the film was found to be about 81% at 550 nm. The obtained high transmittance confirmed the good optical quality of the NiO film and could be used in solar cell applications.The optical band gap E_g (direct& indirect) can be calculated from the plot made between $(\alpha h\nu)^2$ and $(\alpha h\nu)^{1/2}$versus photon energy ($h\nu$) which are shown as Figure 2(b) and 2(c). The relation between absorption coefficient and photon energy is given by theTauc's relation,

$$\alpha h\nu = A(h\nu - E_g)^n \quad (5)$$

where*h* is the Planck constant, ν is the frequency of radiation, E_g is the energy gap and *n* is a constant which represents the nature of transition. The value of *n*is ½ and 2 respectively,for allowed direct and indirect transitions. The calculated optical direct and indirect band gap energies of the prepared NiO thin film was found to be 3.61eV and 1.90 eV respectively.

Optical Properties – PL Analysis

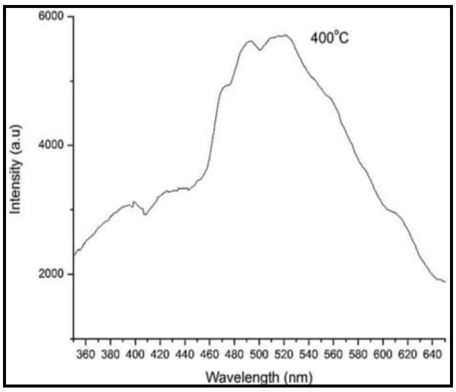

Figure 3 Room temperature PL spectra of NiO thin film annealed at 400°C

Figure 3 shows the room temperature PL spectra of thermally evaporated NiO thin film annealed at 400°C. The PL study indicates that for an excitation wavelength of 290 nm a broad emission peak at 495 nm and shoulder peaks at 390 nm and 430 nm was observed.

The origin of the main strong peak at 495 nm was attributed to the electronic transitions of $Ni^{2+}$and O^{2-} ions. The shoulder emission peaks might be attributed to oxygen related defects.

The type of conductivity of the NiO film annealed at 400°C was determined by the investigation of hot probe technique. That shows the nature of the NiO film to be *p*-type. This *p*-type NiO can be used as a promising active layer for solar cell application.

Conclusion

NanocrystallineNickel oxide (NiO) thin films has been successfully deposited by thermal evaporation method. For the obtained NiO film, the structural and optical properties wereinvestigated by X-Ray diffraction (XRD), UV-Visible and Photoluminescence (PL) spectral studies. The XRD analysis revealed that the film exhibited cubic structure with dominant (1 1 1) orientation. The transmittance of the NiO films was 81% at 550 nm wavelength. The direct and indirect band gaps derived from Tauc's plot are 3.61 eV and 1.90 eV respectively. The room temperature PL spectrum of the NiO thin film was observed in visible region and it originates from electronic transition of Ni^{2+} and O^{2-}ions. These structural and optical study results suggest that the *p*-type NiO thin film coated by thermal evaporation technique is suitable for solar cell applications.

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