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Effect of Substrate Temperature on the Structural, Optical and Electrical Properties of Electron Beam Evaporated NIO Thin Films

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Abstract: *Nickel oxide (NiO) thin films have been deposited onto glass substrates by electron beam evaporation of NiO target and investigated the influence of substrate temperature on the properties of the films. The structural properties of these films were studied by X-ray diffraction technique and different micro structural parameters such as lattice constants and grain size were determined.The optical band gap of the films increased from 3.62 to 3.87 eV with the increase of substrate temperature. The electrical resistivity of the films decreased from 121.8 to 0.074Ωcm with increasing the substrate temperature.*

Keywords: *NiO thin films, structure, bandgap, electron beam evaporation and Raman studies*

1. INTRODUCTION

NiO films have a wide range of applications due to their excellent chemical stability as well as optical, electrical and magnetic properties [1].They have been used as *p*-type transparent conducting films inelectrochromic devices [2, 3], and as a functional sensor layer for chemical sensors [4]. The optical disc of recording material is the new application of NiO films. The optical constants (refractive index *n* and extinction coefficient *k*) and the substrate temperature are the important parameters that affect the performance of an optical film in an optical system [5] and the optical simulation results are strongly dependent on the optical constants of the films [6]. NiO thin films have been deposited by different techniques, including chemical self-assembling [7], sol–gel [8], RF sputtering [9], DC sputtering [10] and recently pulsed laser deposition (PLD)[11–13]. Preparation methods are essential for determining the microstructure and consequently the functional properties of synthesized structures. In this work, electron beam evaporation method was used for the deposition of NiO thin films at different substrate temperatures. The effect of substrate heating during deposition on the structural, electrical and optical properties was studied.

2. EXPERIMENTAL

NiO films were grown on glass substrates by using electron beam evaporation of high-purity (99.9%) NiO pellets. A 10 mm diameter NiO pellet was used as a source target for evaporation. The NiO target was placed in copper crucibles and kept in the water-cooled copper hearth of the electron gun for evaporation. The substrates were placed normal to the evaporation source at a distance of about 50 mm. Before deposition, the material was slowly outgassed with a shutter blocking the vapour from the sample surface. For different purposes of film characterization, the films were deposited different substrate temperatures (Ts). The deposition parameters maintained during the preparation of NiO films are given in Table 1. The structural properties of the films were analyzed by Seifert 3003TT X-ray diffractometer, using Cu Kα radiation (k = 0.1546 nm). The optical band gap of the films was determined using Perkin Elmer Lambda 950 UV-Vis-NIR spectrophotometer. The electrical properties of the films were analyzed by using standard four-probe method.

Table 1. *Deposition parameters of NiO thin films*

Parameters	Values
The target to substrate distance	50mm
Base pressure	6.6×10^{-5} Pa
Working pressure	2×10^{-4}Pa
Substrate temperature	RT to 723 K
Evaporation time	10 min
Accelerating voltage	5kV
Filament current	120 mA

3. Results and Discussion

3.1. Structural Properties

Fig 1 shows the XRD pattern of the NiO films deposited at various substrate temperatures.The crystal structure of the films was identified to be polycrystalline with cubic structure.The films prepared at room temperature exhibited (200) orientation. As the substrate temperature increased to 423 K, an additional peak of (220) appeared along with (200). On further increasing the substrate temperature to 523 K the intensity of the (220) peak was increased and becomes sharper and the (200) peak was disappeared. A decrease in the intensity of the (200) peak with increasing substrate temperature was previously reported by Fujji et al [14]. When the films formed at higher substrate temperature of 723 Kanother peak with increased intensity was observed along (111) orientation and the intensity of the (220) peak was decreased. The orientation of the films was thought to be dependent on the mobility of adatoms and clusters on the substrate [15]. The films deposited on un heated substrate has low atomic mobility and tends to form preferred orientation along (200)orientation. On increasing the substrate temperature, adsorbed atoms gain extra thermal energy and have the motivity to move to another preferred sites along (220).

The lattice parameter of the films increased from 0.4174 to 0.4191 nm with increasing the substrate temperature from 423 K to 573 K there after it decreased to 0.4184 nm at 723 K for (220) peak. The variation in the lattice parameter with substrate temperature was due to the stresses developed in the films [16]. From the XRD results the orientation of grains were mixed mainly (200), (220) and (111). The grain size of the films increased from 12.74 nm to 31.04 nm as the substrate temperature increased from 423 K to 573 K there after it decreased to 17.45 nm at 723 K for (220) peak. The decrease in the grain size of the NiO films deposited at substrate temperature of 723 K may be due to decrease in the crystallinity of (220) peak.

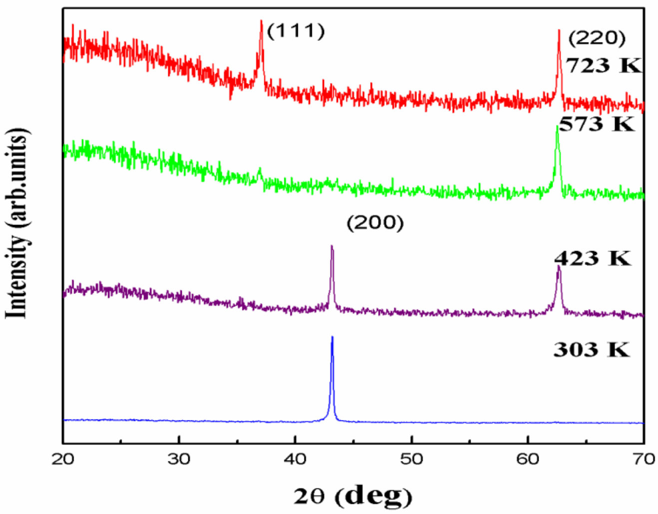

Fig 1. *X-Ray Diffraction Patterns of Nio Films Deposited at Different Temperatures.*

3.2. Raman Studies

Fig.2 shows Raman spectra of NiOfilms grown on glass substrates at temperatures ranging from 303 K (RT) to 723 K. In the Raman spectra of film deposited at (RT) 303 K can be found very weak peak at 300 (cm^{-1}), 580 (cm^{-1}) and another peak at 800 (cm^{-1}). These features can be assigned to the polycrystalline nature of the film. The strong Raman scattering in these films is obviously related to the high phonon density of states in the polycrystalline phase.However, the films deposited at a substrate temperature of 423 K, 573 K and 723 K showed Raman peaks which are located around 580 and 800 cm^{-1} in the range of 100–900 cm^{-1}.The former peak can correspond to the one-phonon (1P) longitudinal optical (LO) phonon modes of NiO and the latter peak can be assigned to two-phonon (2P) 2LO modes [17].By increasing substrate temperatures Raman shift take place because In order for the vibration of the nuclei to interact with this oscillating (accelerated) charge polarization and produce a Raman shift and at high temperatures agglomeration taking place.

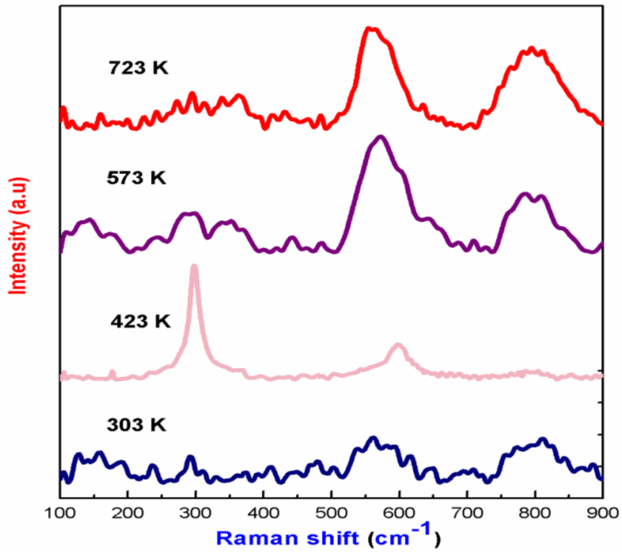

Fig 2. *Raman spectra of NiO films deposited at different substrate temperature*

3.3. Optical Properties

Fig. 3 shows the variation of $(\alpha h\upsilon)^2$Vshυ of samples deposited at various substrate temperatures. It is known that the correlation between absorption coefficient a and optical band-gap $E_g$can be determined by the following equation,

$$(\alpha h\upsilon)^2 = h\upsilon - E_g$$

Where α is the absorption coefficient, A is a constant, and hυ is the photon energy. Hence, the optical band gap for the absorption peak can be obtained by extrapolating the linear portion of the plot of $(\alpha h\upsilon)^2$Vshυ to $\alpha = 0$ (Fig. 4). The value of $E_g$varies in the range 3.56 to 3.88 eV as the substrate temperature increases from RT to 723 K. The change in the optical band gap is due to the change in stoichiometry and crystallinity in the film.

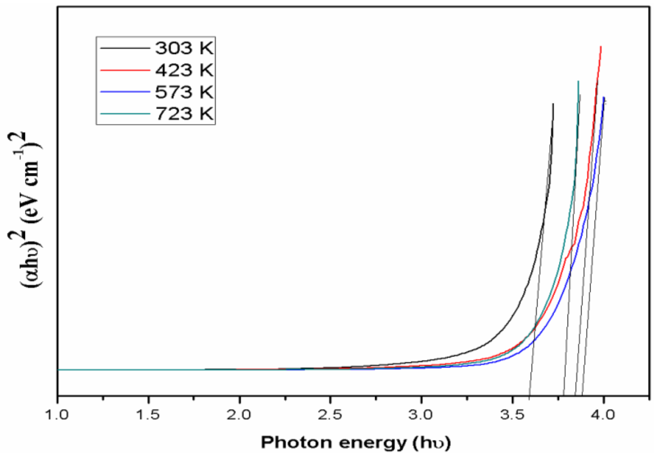

Fig3. *The variation of $(\alpha h\nu)^2$ with photon energy of NiO films deposition at different*

3.4. Substrate Temperatures

Electrical Properties: The electrical resistivity of NiO thin films has a strong dependence on the microstructural defects existing in NiO crystallites, such as nickel vacancies and interstitial defects [18]. Fig.4. shows the electrical resistivity of NiO films as a function of substrate temperature. It was clear that the electrical properties of NiO thin films were greatly affected by substrate temperature. The films showed high electrical resistivity of 121.8 Ωcm at a substrate temperature of 303 K. The electrical resistivity of the films gradually decreased to 7.4 x 10^{-2}Ωcm with increasing the substrate temperature to 723 K. This decrease in electrical resistivity was due to increase in carrier concentration.The Hall mobility measurements indicated that the films were p-type conduction. The Hall mobility of the films increased from 1.8 to 7.6 $cm^2V^{-1}s^{-1}$ with increasing the of substrate temperature from 303 to 723 K.

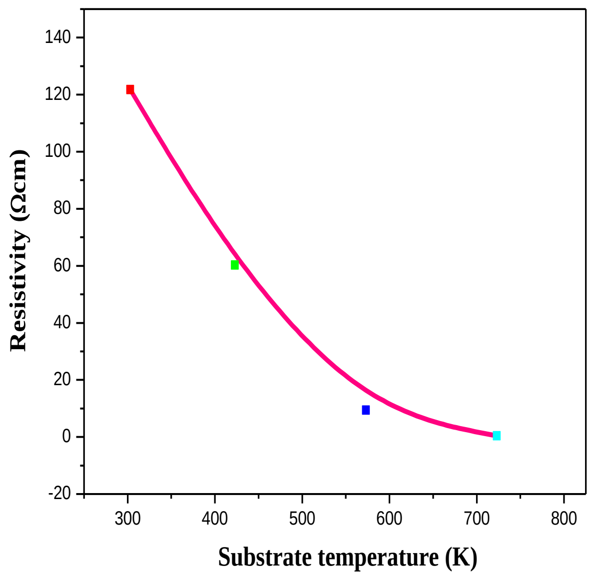

Fig 4. *Change of electrical resistivity of NiO films as a function of substrate temperature.*

4. Conclusion

NiO thin films were deposited on to chemically and ultrasonically cleaned glass substratesatdifferentsubstrate temperatures by using electron beam evaporation. The optical band gapincreaseswith increasing the substrate temperature. The structural parameters of a thin film largely depend on the preparation method and conditions. The structural properties of these films were studied by X-ray diffraction technique and different micro structural parameters such as lattice constants and grain size were determined. The optical band gap of the films increased from 3.62 to 3.87 eV with the increase of substrate temperature. The electrical resistivity of the films decreased from 121.8 to 0.074Ωcm.

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