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Physical Characterization of Antimony Doped Nanostructured Nickel Oxide Thin Films



Abstract: - Antimony Doped NiO and nanostructured NiO films were produced using Simple Spray Pyrolysis (SP). The anticipated films were polycrystalline, with a favored peak along the (200) plane, according to an XRD examination. The grain size had decreased from a maximum of 17.81 nm to 28.49 nm at 3% antimony doping. Calculations were made for micro strain and dislocation density, among other microstructural characteristics. Findings came in. The morphology of the surface (AFM) of the film is affected by this antimony. The (Undoes) nanoparticles' average particle sizes were discovered to be 87.5, 49.7, and 41.6 nm. NiO: (Ra) and (Rrms) of AFM: NiO, undated NiO, NiO with 1% Sb, and NiO with 3% Sb, respectively Sb films have a wavelength range of (10.71-5.26) nm and (8.76 - 3.32 nm). Using UV-visible transmission spectroscopy, it was discovered that the deposited films are transparent in the visible spectrum. The refractive index and extinction coefficient both decrease with antimony concentration and the energy gap was 3.63–3.52 eV.

Keywords: NiO, Sb, thin films, XRD, Morphology, Optical Properties, band gap

I. Introduction

NiO is a p-type film because of its excellent properties, which include great chemical stability, strong crystal clear, a direct energy gap of 3.6–4.0 eV, a high transparency spectrum, and a low material cost [4]. By increasing the quantity of interstitial oxygen and/or Ni vacancies when NiO is present, the resistivity of undated NiO films is dramatically decreased [5,6]. The stoichiometric balance between the nickel and oxygen atoms has a big impact on the behavior of NiO. They go through a variety of modifications as a result of their nonstoichiometric, which have a variety of effects on a variety of applications, including organic light-emitting diodes [11], electrodes in solar cells [8, 9], gas sensors [10], and electro chromic materials [7]. There are several different types of nickel oxide, including NiO, NiO₂, NiO₄, and Ni₂O₃. Bulk NiO has a high melting point (2000 °C) and a very high resistivity, indicating that high-temperature applications are possible for it. Because Ni²⁺ vacancies are created in the NiO structure when heated in air, NiO exhibits p-type semi conductivity [12]. NiO films were produced using a comprehensive various techniques, such as reactive sputtering [13], PECVD [5], EBE [6], sol-gel [14] and SP [15-17]. Compared to the other technique, the spray pyrolysis method is much simpler, less expensive, safer, and less expensive overall as a non-vacuum system of deposition method [4]. This method is used to manufacture transparent conducting oxides. Spray pyrolysis has several benefits over

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traditional pneumatic spraying, the most notable of which are its reduced material consumption, improved capacity to regulate moderate carrier gas circulation and splash, all of which make it possible to deposit very thin layers of a steady thickness [18]. In this paper, we started into how antimony affected the characterization of NiO thin films, which is essential for a more profound comprehension and improvement of the material quality.

II. EXPERIMENTAL

A spray pyrolysis coating unit was incorporated inside the device to deposit NiO and NiO: Sb thin films. The right proportions of nickel chloride (NiCl₂) (0.1M) dissolved in deionized water were combined to create the spray solution. Antimony dichloride (SbCl₃) was resolved in a solution of is then incorporated into the combination to accomplish Sb doping. The doping concentration of (0, 1, 3%). The conditions for preparation: In order to prevent cooling, the spraying period of 10 seconds was extended by 100 seconds. The base temperature was 400°C, and the vehicle gas used was nitrogen. A measuring method was implemented to determine the the movie's dimension, which came out as being 340±25 nm. Using a UV-visible shiatsu double beam spectrophotometer, optical transmittance spectra for as-deposited thin films were evaluated. The nature of film structure was ascertained using XRD, and film surface was examined using AFM.

III. RESULTS AND DISCUSSIONS

Fig. 1 shows the anticipated movie' XRD styles. All the films were polycrystalline. At 37.32°, 43.28°, and 62.70°, respectively, peaks were visible that were attributed to the (111), (200), and (220) planes. These features a typical JCPDS card No (04-0835) [19, 20]. The direction of (200) showed a clear peak, well supported by other researchers [21].

Scherer's equation is applied to make a prediction of the grain size, denoted by "D." [22-24]:

$$D = \frac{0.9\lambda}{\beta \cos\theta} \quad (1)$$

Where λ is X-rays intensity, β is (FWHM).

According to Table 1, D for NiO and NiO: 3% Sb films are 17.81 nm and 28.49 nm, respectively. As antimony doping levels rise, grain size increases due to grain growth [25, 26].

The dislocation density (δ) was calculated by Eq. 2 [27-29]:

$$\delta = \frac{1}{D^2} \quad (2)$$

The strain (ϵ) is gained via the relation [30-32]:

$$\epsilon = \frac{\beta \cos\theta}{4} \quad (3)$$

The structural parameters S_{para} are display in Table 1. Increasing the amount of doping with antimony results in a reduction of the value of strain [33, 34]. Figure (2) lists S_{para} against Antimony content.

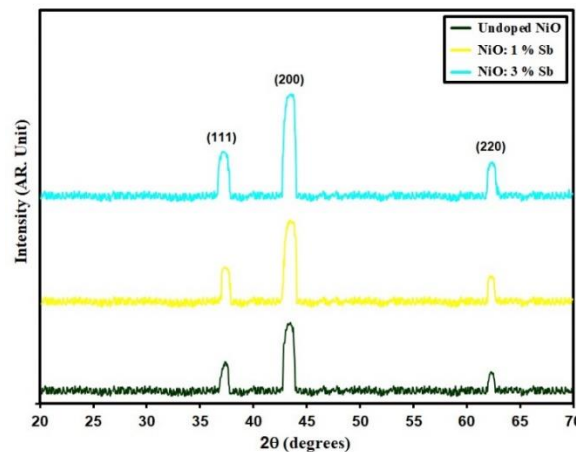


Fig. 1 XRD styles of grown films.

The surface abrasiveness and root-mean-square of the planned films are examined using AFM images. Crystallites with regular sizes and dense packing are visible in Fig. 3's AFM scans. For the necessary films, the typical Pav particle diameter was 87.5, 49.7, and 41.6 nm. undoped NiO and NiO: Sb films exhibit roughness on the surface (Ra) and root mean square roughness (Rms) in the range of (10.71-5.26) nm (8.76-3.32), respectively, according to AFM. Ra has decreased as a result of increased grain output [35–37]. In Figure 3, Ra and Rms are shown. The Ra and Rms with antimony content are displayed in Table 2.

TABLE 1. Grown-up flicks D, Eg, and Spara.

Sample	2 q (°)	(hkl) Plane	β (°)	Eg (eV)	Grain area (nm)	disconnection density (δ) ($\times 10^{14}$) (lines/m ²)	shear(ϵ) ($\times 10^{-4}$)
Unreval NiO	43.28	200	0.48	3.63	17.81	31.52	19.46
NiO: 1% Sb	43.25	200	0.42	3.56	20.35	24.14	17.03
NiO: 3% Sb	43.21	200	0.36	3.52	2849	12.16	12.16

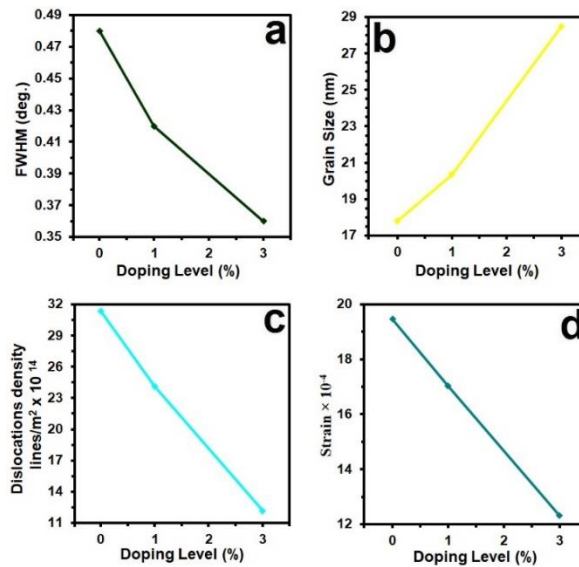


Fig. 2 Spara of the deliberate feature.

TABLE 1. AFM parameters of grown films.

Samples	Pav nm	Ra (nm)	Rms (nm)
Undoped NiO	87.5	10.71	8.76
NiO: 1% Sb	49.7	9.47	6.32

NiO: 3% Sb	41.6	5.26	3.32
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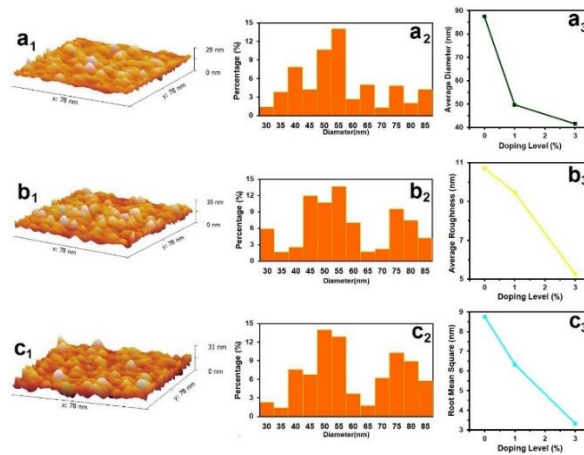


Fig. 3 AFM results of grown films

In Fig. 4, optical characteristics of the intended films doped with antimony at 1% and 3% are depicted. With antimony doping, the transmittance (T) spectra showed a decrease. This suggests that the addition of Antimony to the films affects their optical properties [38,39].

The absorption coefficient (α) is gained by Eq.4 [40-42]:

$$\alpha = \frac{\ln (1/T)}{d} \quad (4)$$

Where d is film thickness. Figure 5 illustrates a shift in α . In the visible range of the wavelength, all films show a high absorption coefficient with a value of 10^4 (cm^{-1}), indicating a direct transition [43, 44]. As antimony content rises, the absorption coefficient rises as well.

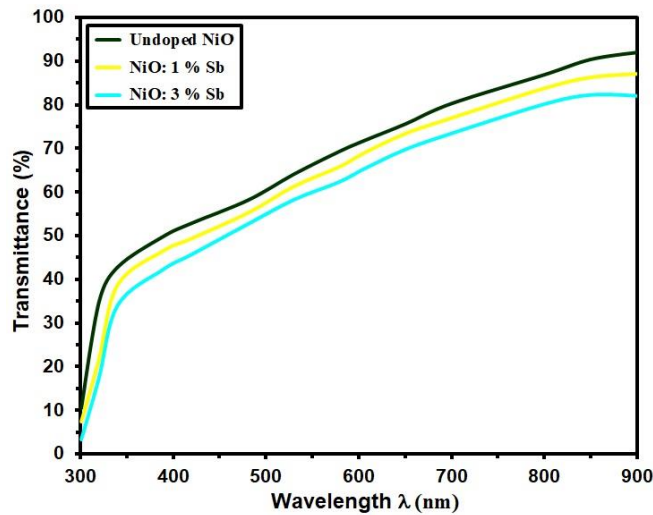


Fig. 4 T of the grown films.

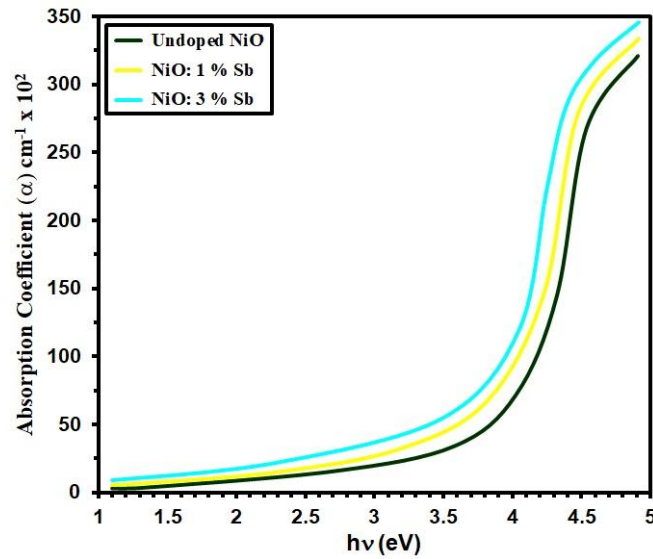


Fig. 5 α Vs $h\nu$ of the prepared films.

Tauc's relation can be used to evaluate the bandgap energy E_g [46-48]:

$$(\alpha h\nu) = A(h\nu - E_g)^{\frac{1}{2}} \quad (5)$$

where A is a constant, Fig. 5. displays that When antimony concentration increased, the energy gap for all produced films reduced. The energy difference ranged from 3.63 to 3.52 eV [49, 50].

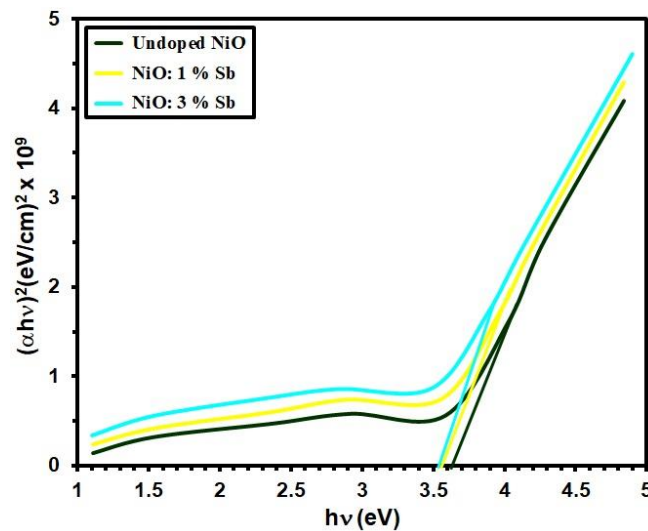


Fig. 6 E_g of the intended films.

The calculated value of (α) was gained to estimate the values of the extinction coefficient (k) utilizing the relation [51-53]:

$$k = \frac{\alpha\lambda}{4\pi} \quad (6)$$

Where λ is the wavelength. For all the films under investigation, Fig. 7 depicts the extinction coefficient's dependency on wavelength. It is evident that when the doping Antimony proportion increases, the extinction coefficient decreases [54, 55]. an approach to determining the value of the refractive index (n) is to make use of the reflectance (R) spectrum [56-58]:

$$R = \left(\frac{n - 1}{n + 1}\right)^2 \quad (7)$$

The value of n was determined by applying the formula below [59-61]:

$$n = \frac{1 + \sqrt{R}}{1 - \sqrt{R}} \quad (8)$$

All films displayed comparable behavior in the refractive index spectra, as seen in Fig. 8. It is evident that n decreases as the amount of doped antimony increases [62, 63], The density and surface roughness are to blame for the refractive index's small decrease [64, 65].

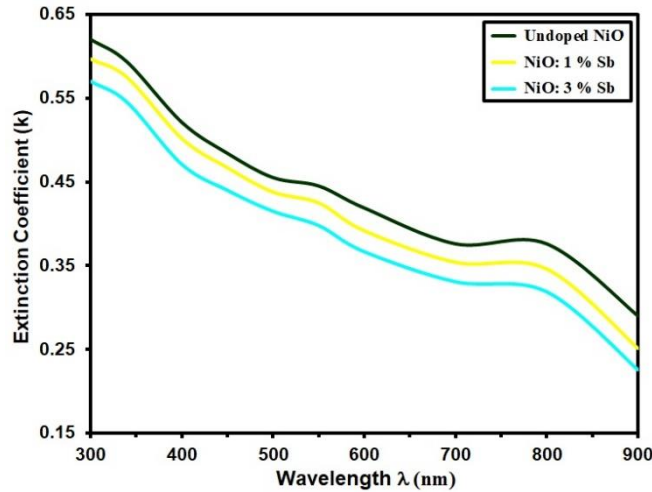


Fig. 7 k of the grown films.

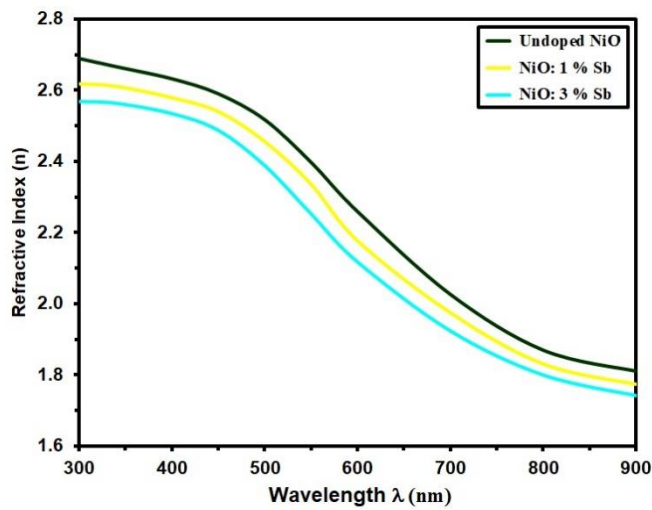


Fig. 8 n for grown films.

IV. CONCLUSION

The nanostructured matter undoped NiO and NiO: Sb thin films were made using a low-cost plasma pyrolysis method. NiO and undoped NiO: Sb. XRD patterns reveal that the samples are polycrystalline with a preferred (200) orientation. The generated films with XRD measurements showed grains between 17.81 and 28.49 nm, misfit densities between 31.52 and 12.16, and strains between 19.46 and 12.16. The median diameter for the doped samples was discovered to be (87.5), (49.7), and (41.6) nm, respectively. The transmittance decreases as arsenic concentration increases. The optical band gap value reduces from 3.63 eV to 3.52 eV when antimony concentration increases, although n and k increase.

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