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Effect of Boron Doping on Structure, Topography and optical properties of nickel oxide Thin Films by spraying technique

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Abstract

NiO thin films were grown via chemical spray pyrolysis (CSP) technique . X-ray diffraction (XRD) styles showed cubic phase and dominant direction at (200). The crystallite size values increase from (13.53 to 15.83) nm via B content . AFM results indicate a smooth surface with RMS roughness from 7.65 nm to 4.92 nm of Undoped NiO, NiO: 2% B and NiO: 4% B. AFM image displays that particle size was in the region of 56,61 nm to 41,87 nm with NiO and NiO: 4% B respectively. It is found that the bandgap decreases as the B content increases from 3.5 eV to 3.4 eV for NiO: B thin films. optical constants were also obtained. These results proved the ability of use these films in solar cells.

Keywords: NiO; B; thin films; CSP; Structure; topography; Optical Properties; bandgap.

Introduction

Metal oxide materials are very important in industrial applications because the wide band gap makes these materials suitable in electronics applications [1-7]. Numerous applications require transparent, conductive coatings for its unique properties [8]. NiO is a remarkable antiferromagnetic with band gap of 3.15- 4.0 eV [9,10]. Several properties of NiO films altered due to their non-stoichiometry, and these variations led to different applications, including electrochromic display devices, chemical sensors, transparent electronic devices [11–14]. NiO films was grown by various methods, like EBE [15,16], sputtering [17], reactive PLD [18,56-76], electrochemical deposition [19] and spray pyrolysis [20-27]. In this work CSP was adopted to study physical properties of the prepared NiO:B films.

Experimental

NiO films were prepared utilizing 0.1 M of $NiCl_2$ resolved in 1:1 redistilled water and ethanol. Boron trichloride resolved in redistilled water to get the intended doping , slight drops of HCl were joined the solution to get it fine . CSP was employed to prepare NiO:B film. The optimum conditions are: base temperature was 400 ^{O}C, space between spout and base was 28 cm, spraying interval 8 s hold by 60 s to evade cooling, spray rate was 4ml/min, and N_2 is offered as carrier gas. Film thickness is obtained utilizing weighing method to be 325 ± 25 nm. CdO thin film formed was confirmed by XRD analysis. AFM was utilized to obtain film topography.UV-Visible spectrophotometer was utilized to record the transmittance spectra.

Results and Discussions

XRD styles display that thin films are cubic . The observed 2θ value of the deposited NiO and NiO:B films were compared with the ICDD card No (75-0197). The favored orientations are (1 1 1), (2 0 0) and (2 2 0) planes and are in perfect concurred with the standard. B doping in NiO thin films suitably modified the crystalline structure of undoped NiO. An enhancement in peak intensity can be deduced either to the grain growth linked with crystal order.

The crystallite size (*D*) was obtained employing Scherrer formula [28-31]:

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

where λ wavelength of X-ray, θ -Angle of diffraction and β - FWHM. *D* values were in the range of (17.10-20.81) nm.

The dislocation density δ is obtained utilizing the Eq. (2) [32-35]:

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

The value of dislocation density δ decreases from 34.5 to 23.09 increasing Boron content,

The strain ε is calculated using the Eq. (3) [36-39]:

$$\varepsilon = \frac{\beta cos\theta}{4} \qquad (3)$$

The value of parameter decreases from 20.27 to 16.6 increasing Boron content, the obtained structural coefficients are displayed in Table 1. Fig. 2 symbolizes FWHM, *D*, δ and ε versus Cu dopant.

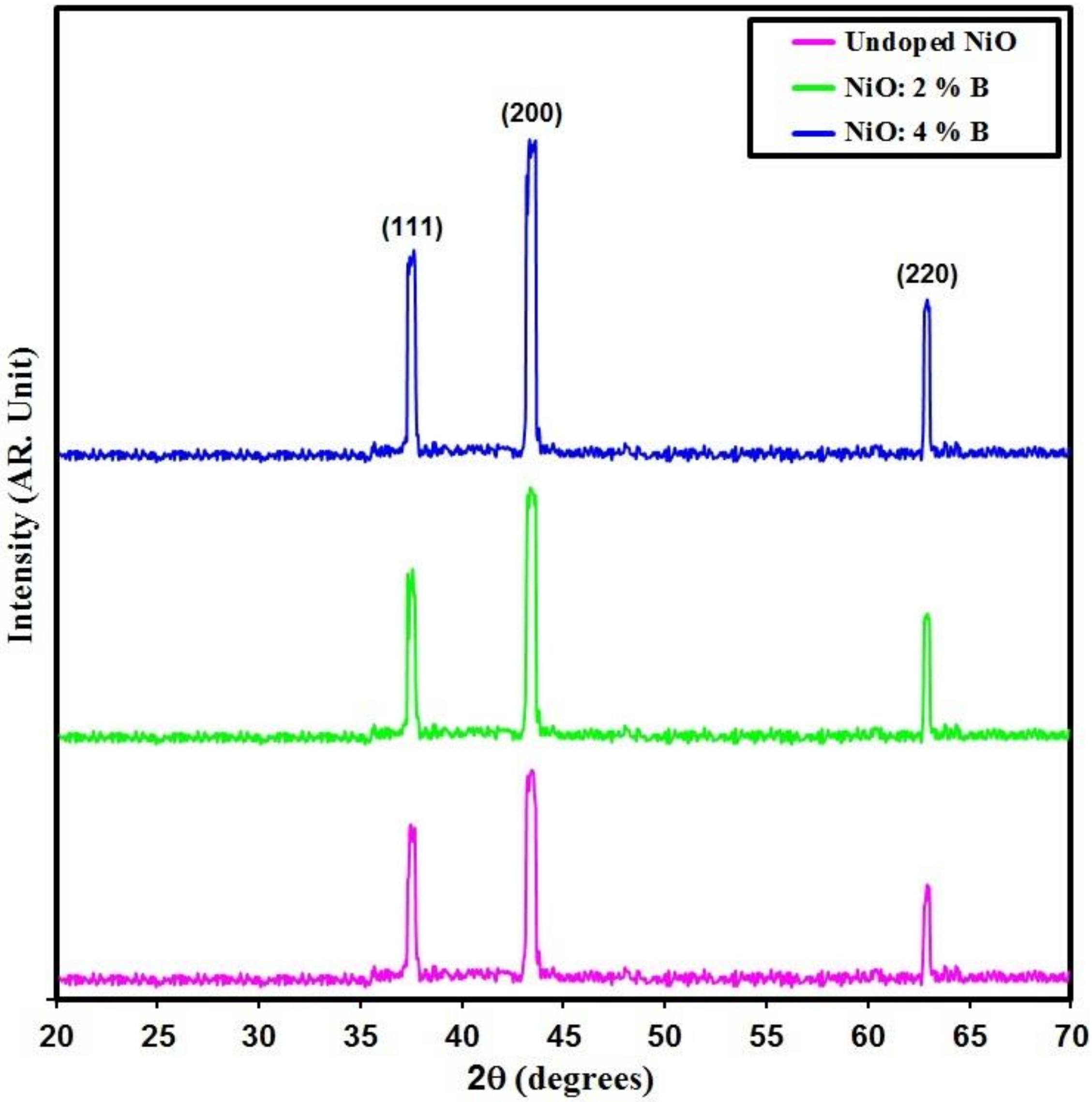

Fig.1. XRD styles of grown films.

Table 1. D, E_g and structural coefficient of the grown films.

Samples	(hkl) Plane	2 □ (º)	FWHM (º)	Optical bandgap (eV)	Grain size (nm)	Dislocations density ($\times 10^{15}$) (lines/m^2)	Strain ($\times 10^{-3}$)
Undoped NiO	200	43.30	0.50	3.50	17.10	34.19	20.27
NiO: 2% B	200	43.26	0.46	3.45	18.58	28.96	18.65
NiO: 4% B	200	43.21	0.41	3.40	20.81	23.09	16.61

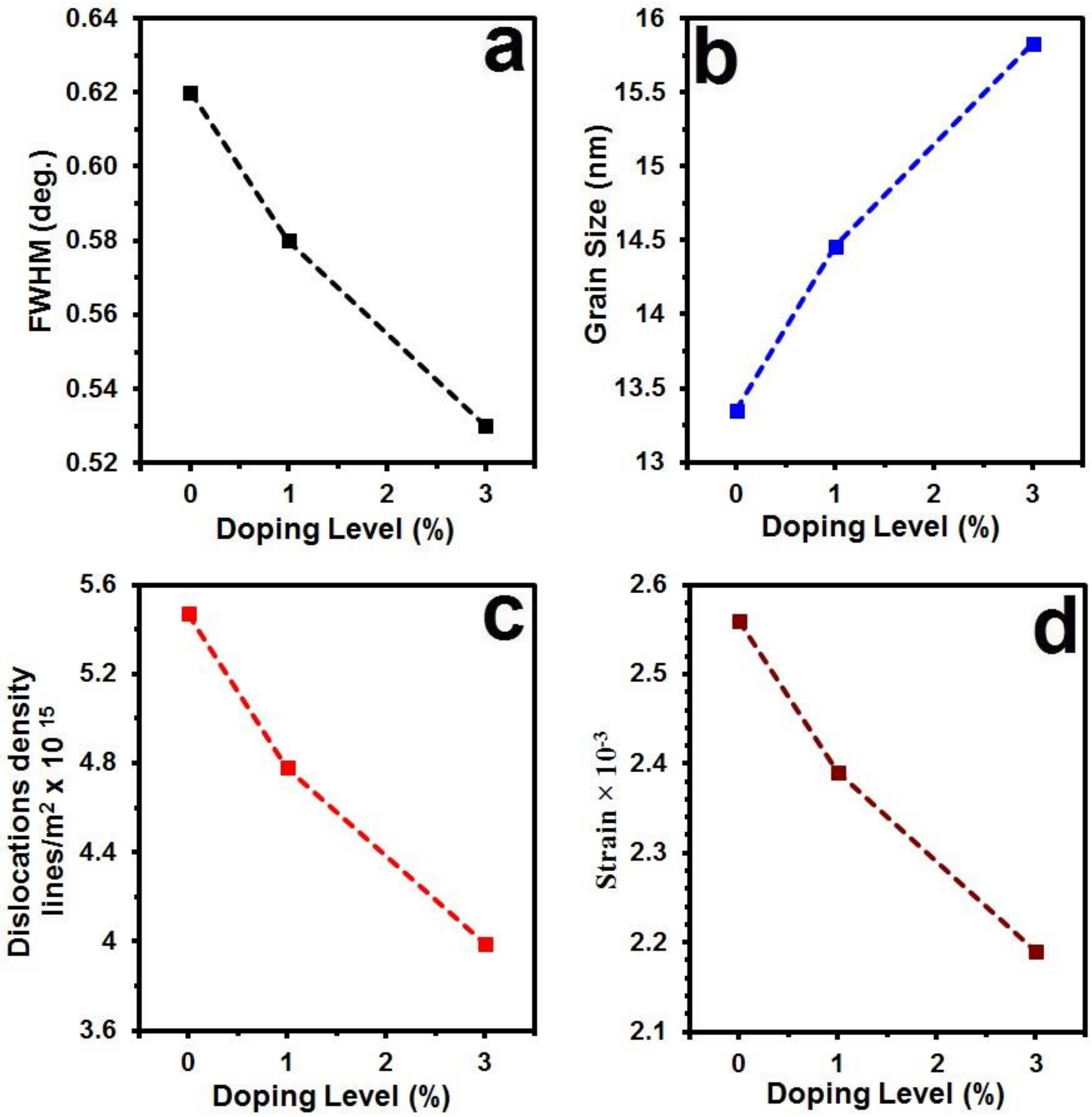

Fig.2. FWHM (a) D (b) δ (c) ε (d) of the intended films.

Surface topography for Undoped NiO, NiO: 2% B and NiO: 4% B were shown by AFM images. Figure 3. Displays the granules ,which exist in films suffer scattered in some zones . surface morphology can be estimated via roughness (Ra) and root mean square roughness (rms). From Figure 3 (a3, b3 and c3). Average Particle size and rms values of (56.61. 47.24 and 41.87) nm and (7.65, 6.78 and 4.29) nm, respectively, which strongly affected by Boron dopant.

Table 2 shows that the average roughness and average particle size P_{av} increases with B content . Surface area increment plays an important role for photocatalytic activity.

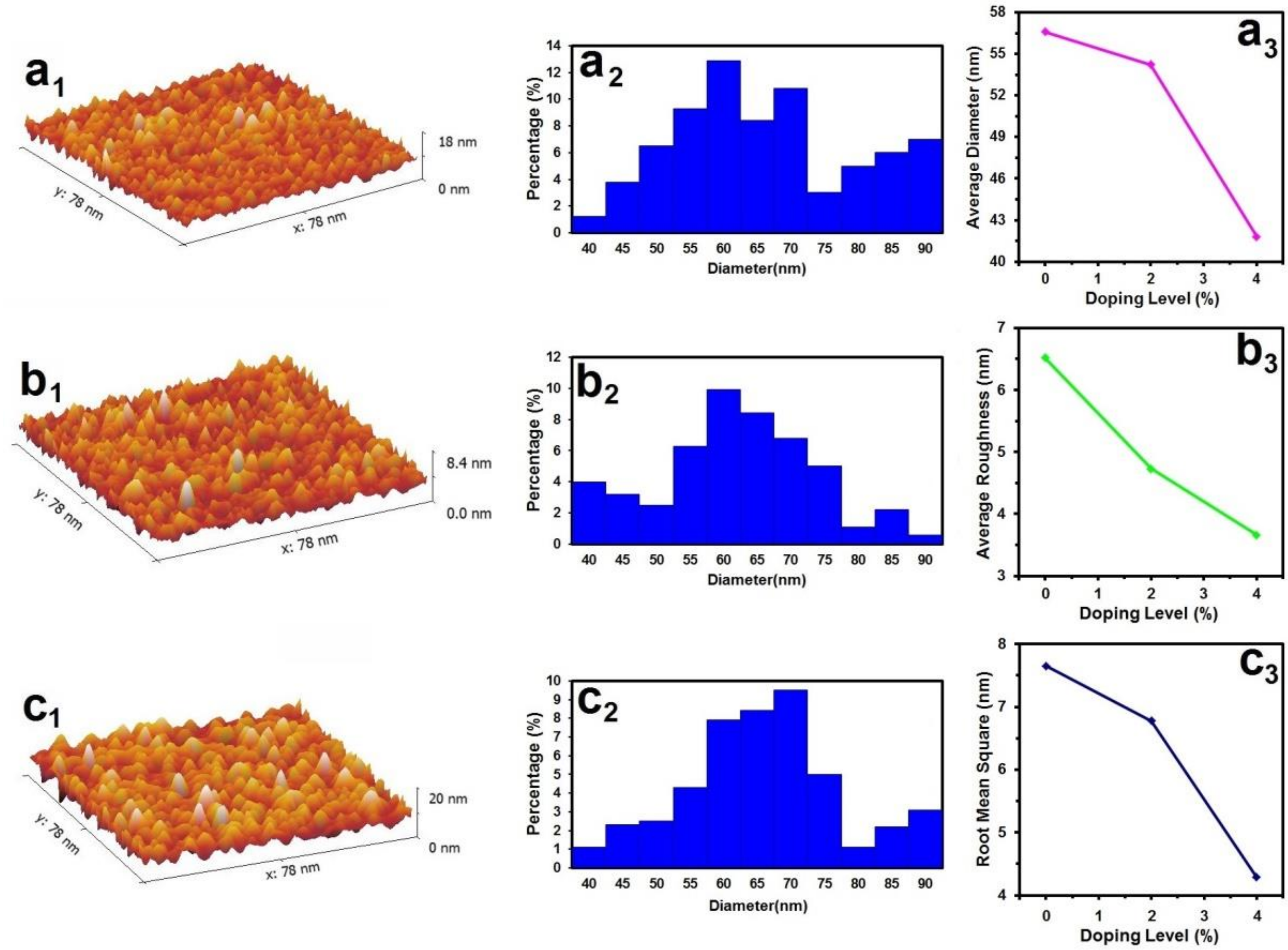

Fig. 3. AFM images (a_1, b_1 and c_1), granularly distributed (a_2, b_2 and c_2) and variance of AFM parameters (a_3, b_3 and c_3).

Table 2. AFM parameters of grown films.

specimen	P_{av} nm	Ra (nm)	rms. (nm)
Undoped NiO	56.61	6.52	7.65
NiO: 2% B	47.24	4.73	6.78
NiO: 4% B	41.87	3.66	4.29

Fig 4 offers that the transmittance spectra of intended films. It was monitored that the highest transmittance value was 68% for NiO.

The absorption coefficient α can be obtained by the following relation [40-43]:

$\alpha = (2.303\times A)/t$ (4)

Where (t) is film thickness. Figure (5) offers α for NiO thin, it is found that α decreases with increase in hν and this attributed to the effect of the Boron.

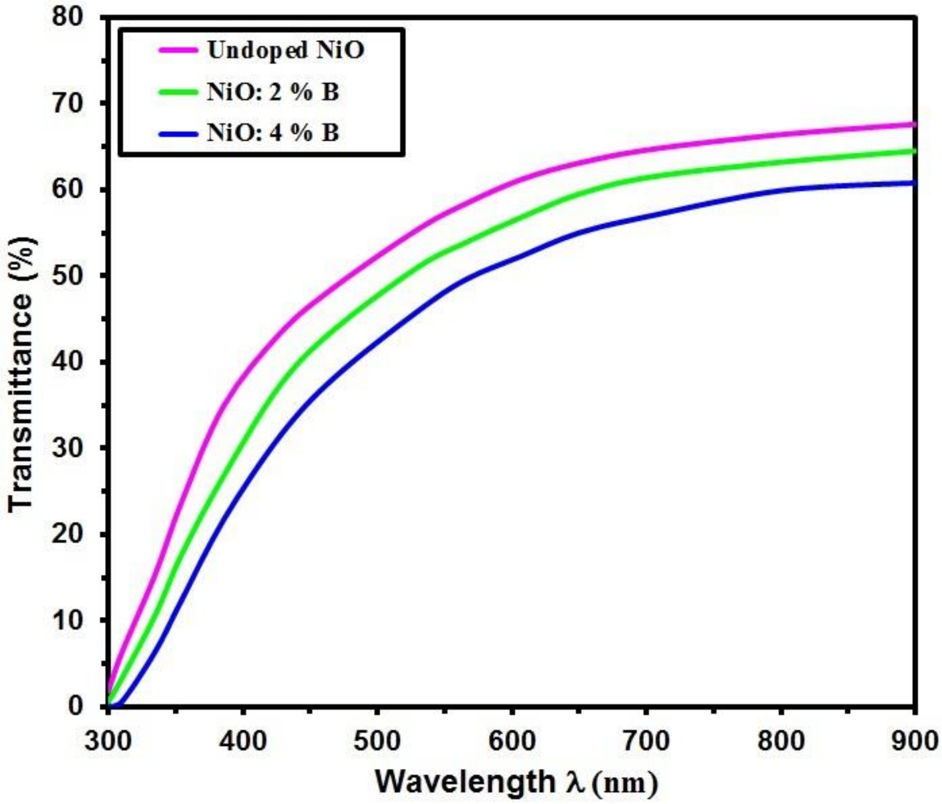

Fig.4: T of the intended films.

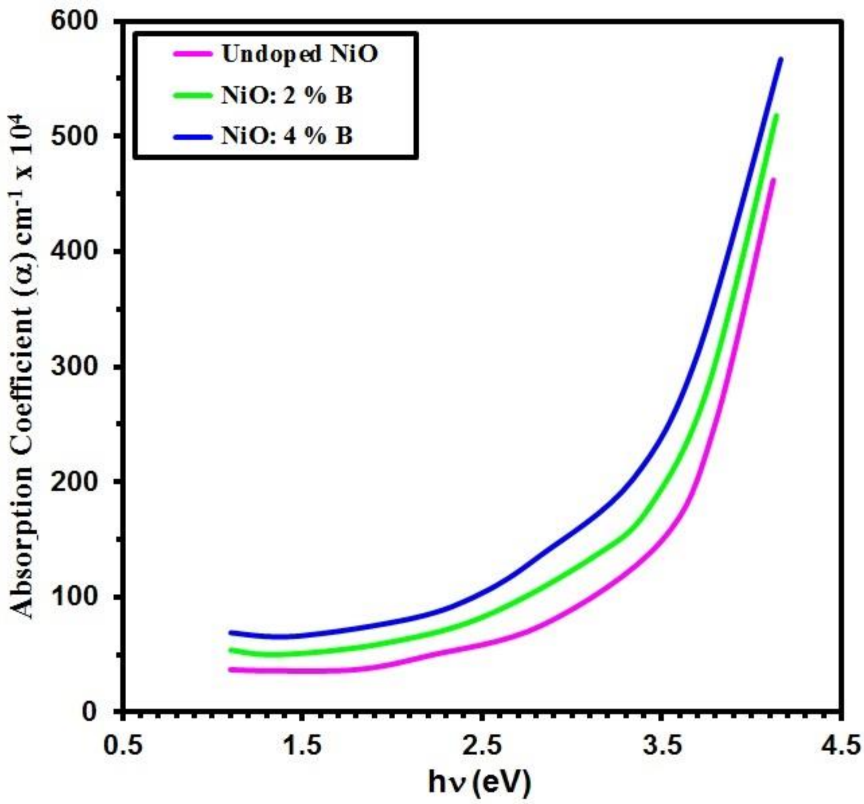

Fig. 5: α against hν of intended films.

The energy gap (Eg) can be obtained from Tauc equation [44-47]:

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

where A is constant, the value $1/2$ which suggest an allowed direct transition [28]. Fig. 6. Display this relation, it can notice that bandgap offer a decrement from 3.50 eV for NiO film to 3.40 eV after 4% added of B in NiO film.

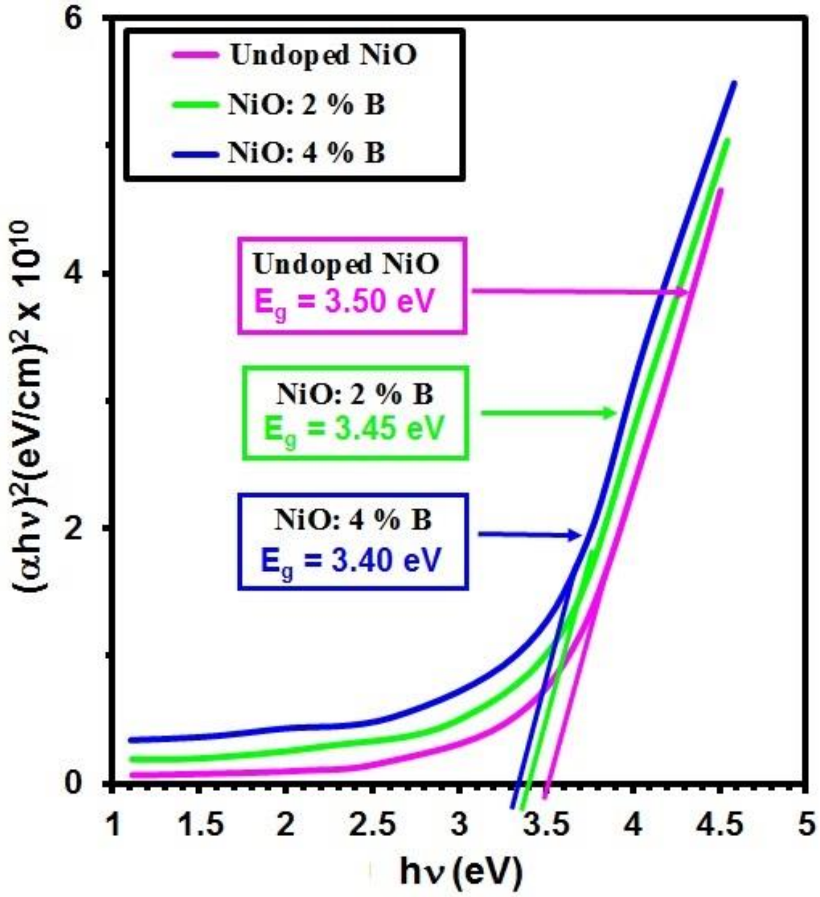

Fig. 6: $(\alpha h\nu)^2$ via hν for grown films.

The extinction coefficient (k), is defined as [48-51]:

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

Fig.7 represent the vaue of k with wavelength. A decrease in k with increasing content of Boron is noticed.
The refractive index (*n*) is obtained utilizing the relation [52-55]:

$$n = \left[\left(\frac{4R}{(R-1)^2}\right) - K_0^2\right]^{1/2} - \frac{R+1}{R-1} \qquad (7)$$

Fig.8 displays the value of n versus wavelength for NiO:B thin film for various B. it is found that n decreases with increment of Boron until 550 nm, thereafter, n altered a bit at λ>550 nm.

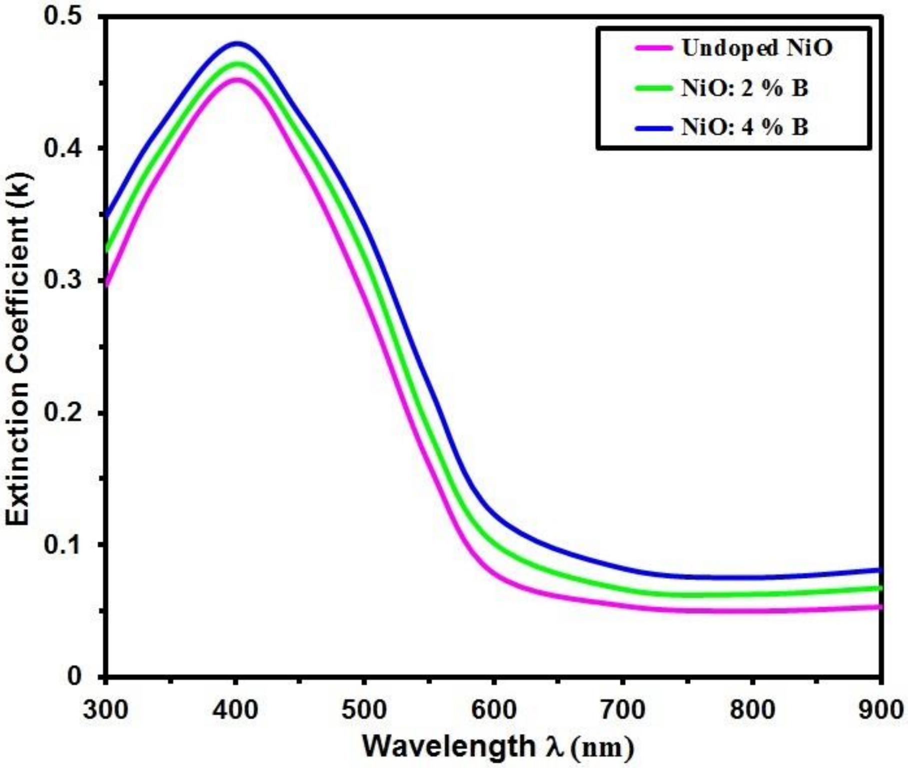

Fig.7: k of intended films.

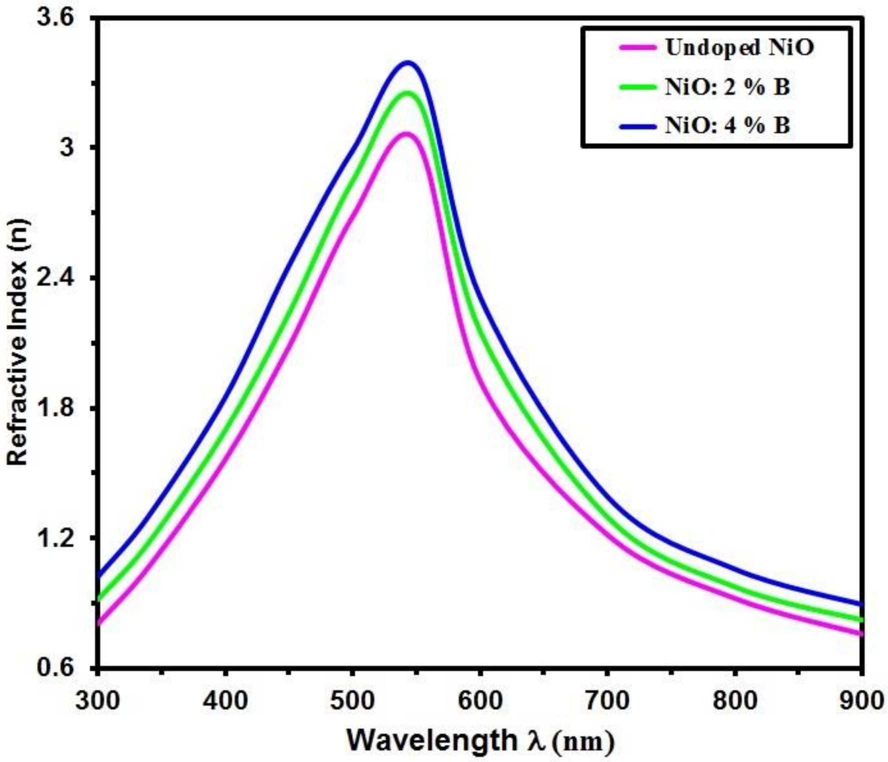

Fig. 8. n of intended films.

Conclusion

NiO and NiO:B films were coated employing CSP method. The effect of Boron Doping on the structural was characterized by XRD and optically via UV-visible. The XRD result offere the polycrystalline nature of grown films. The parameters like grain size , δ and ε were calculated. All the films reveal the most favored orientations along (1 1 1), (2 0 0), and (2 2 0) planes and the structure is confirmed to be cubic, and dominant direction at (200). The morphology of creating of Undoped NiO, NiO: 2% B and NiO: 4% B nanosheets were AFM was investigated. The UV study shows the transmission and absorption spectra with bandgap ranged between 3.50 eV to 3.40 eV. The maximum absorption for the films occurred within the UV region. Transmittance decreases with an increase in the Boron concentration, while α, k , and n are increased with increasing Boron content.

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