



Influence of Li Doping in NiO Thin Films Prepared by Simple Chemical Method

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Abstract

This study deals with the study of the structural and visual properties of NiO and Li Doped NiO films in different percentages (0.02, 0.04, 0.06, 0.08% mol). Thin films of NiO were deposited on glass substrates at 300 ° C and 150 nm using droplet casting technique. X-ray diffraction (XRD) showed that multi-crystalline films had a cube structure with a preferred orientation along the length of (111). The tonic stimulator did not change between 0.02, 0.04, 0.06 and 0.08% Grammy% of the preferred trend. The average grain sizes of crystals classified from XRD data were found in the range of 15.62 - 37.52 nm. Atomic Force Microscope (AFM) data shows that the film surface is extremely smooth. The photovoltaic permeability of pure NiO membranes is 72% in the visual and x-ray regions (NIR), which is important for their applications as window layers in solar cells.

Keywords: Nickel oxide, XRD, AFM, grain sizes, thin film.

Introduction

Semiconductors made of metal oxides have attracted wide attention because of their unique properties and their potential large applications in various manufacturing processes. Nickel oxide is a chemical compound with the NiO formula. It is a transitional metal oxide with a wide gap in the range from 3.6 to 4.0 eV [1]. Nitrogen is a type of anti-viral semiconductor a promising candidate for many applications such as lithium ion batteries, solar cells, anti-magnetic layer, electrochemical capacitors, chemical sensors, and electromagnetic coatings. Stoichiometric NiO at room temperature is an insulator with a resistance of 1013 cm.

Lithium (Li) is an element of group 1 (IA) containing only a single valence electron (1s22s1). Elements of group 1 are called alkali metals. Lithium solid material is only about half the water density and lithium metal is the least dense metal. A small piece of lithium silver, but deformation in a minute or so in the air to give gray surface. Its chemistry dominates its tendency to lose the electron to form me.

In this research, we prepared fine films from pure NiO and NiO doped NiO using droplet casting technique. Li effects on structure and some optical properties of NiO films were studied.

Experimental Work

The nickel oxide solution was prepared from NiCl₂ using a chemical method. Two different bathroom combinations were used. The first is the preparation of pure nickel oxide solution which is achieved by dissolving 7.48g of NiCl₂ with 1m in 50ml of water. They were mixed slowly for 30 minutes using a stirrer magnetic device, then get a pure homogeneous solution, we get the green solution.

The second bath was the same as the first bath with the addition of 0.1M of LiH₂O solution to different concentrations. The rotor spoiler was used to prepare films under speed conditions of 3000 rpm and time of 20 seconds. Then take 20µl of the solution and drop it onto the substrate using a circulating device, dry in an electric oven at 60 ° C for 2 minutes to remove the solvent (water).

Finally this process was repeated four times, to get sample with 30 layers. The samples were annealed by 300C for 1hr using jinyu-

700 device to reduce the crystal defects and increasing the conductivity of the sample.

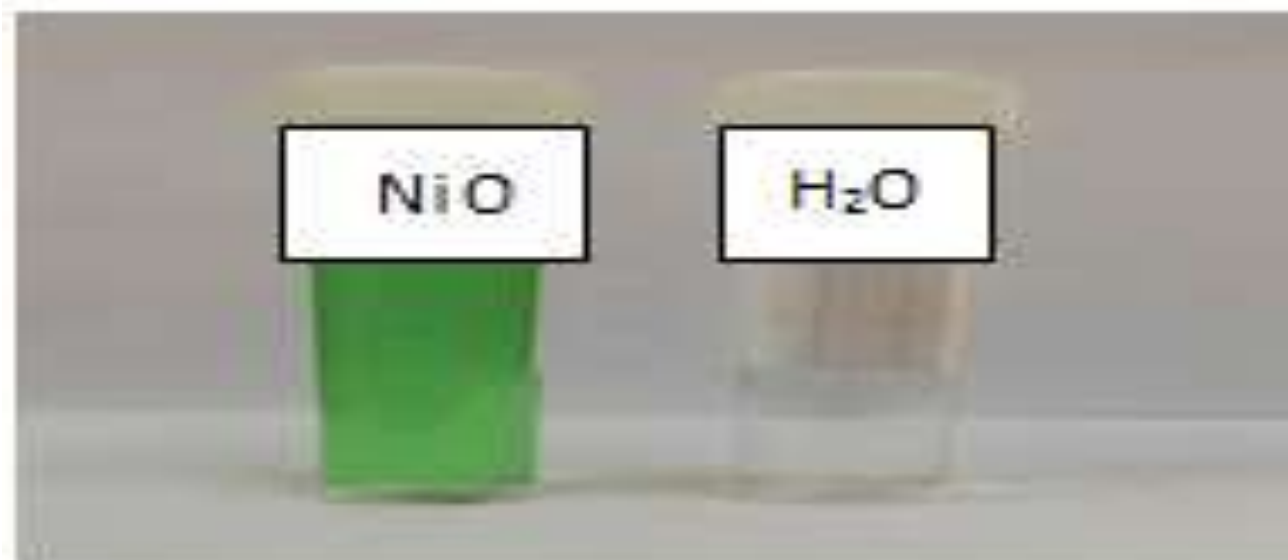


Fig.1: NiO freshly colloidal nanoparticles) which are prepared by chemical (left) which are prepared by chemical method and the solution (right)

Results and Discussion

XRD patterns of the films deposited at a glass substrate temperature 60°C, and thicknesses 150nm are shown in Fig.2. The films of pure NiO and Li doped NiO were found to be polycrystalline in the usual with three diffraction peaks along with (111),(200) and (220) planes of cubic NiO phase (JCPOS 047- 1049).The XRD showed the dominating peak is (111) [7,8]. The results showed that the intensity of the top (111) increases by increasing the concentration of lithium doping compared to the pure NiO. This

confirms that the crystallization rate may decrease due to the increase in the FWHM, except for the (6%Li) Less than all the rate of doping due to the film of crystalline defects in the lattice where the increase in the height of some peaks indication of increasing the crystallization of material and reduce the defects of crystalline atoms give the material potential energy to rearrange itself in the lattice and the FWHM is less, but the rate of doping 8% Li there is no dominant peak in it this means that the crystal structure has become amorphous.

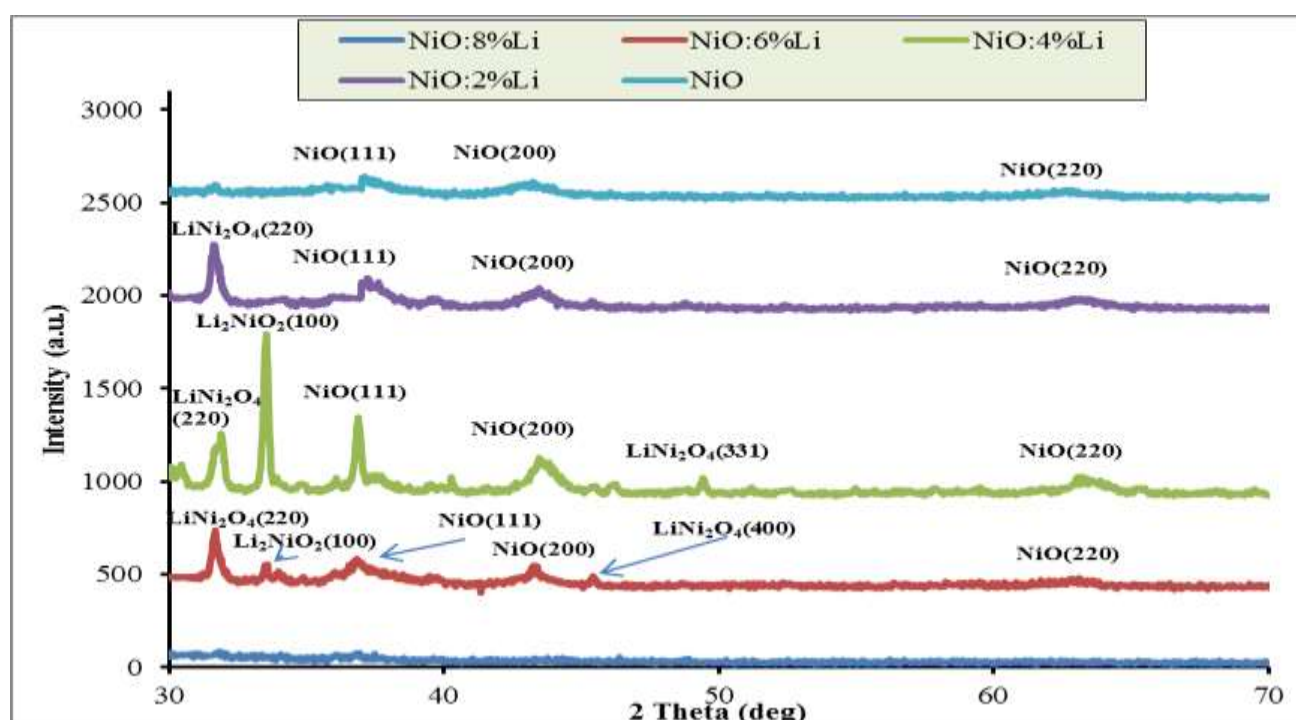


Fig.2: XRD patterns of all prepared films

Table 1: Structural parameters for all prepared films measured at thickness of 150nm

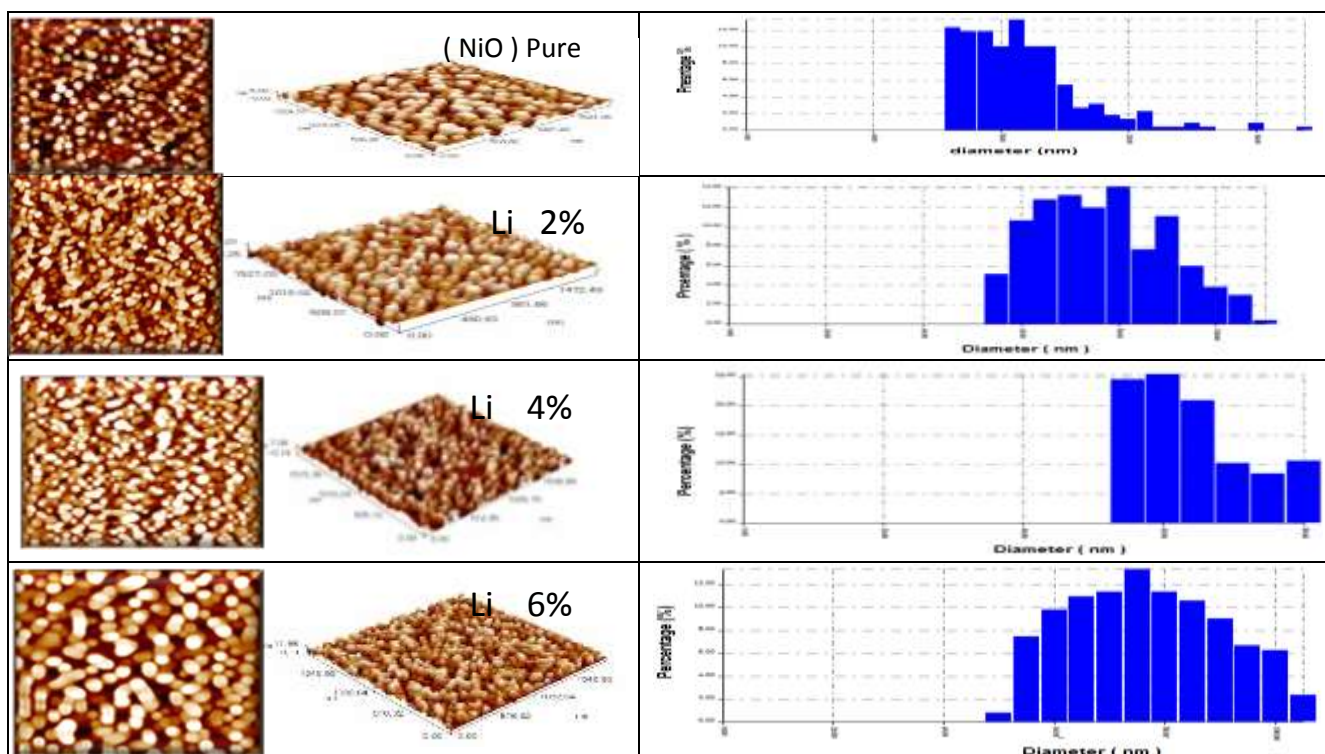
Samples	2 Theta (deg)	(hkl) plans	β (deg)	D_g (nm)	$\eta \times 10^{-4}$ (lines ² ·m ⁻⁴)	$\delta \times 10^{14}$ (lines/m ²)
NiO Pure	37.02	NiO(111)	1.74	4.79	72.32	4792.7
	42.98	NiO(200)	1.6	5.31	65.24	399.3
	62.5	NiO(220)	1.46	6.34	54.65	2736.3
NiO : Li 2%	31.6	(LiNi ₂ O ₄ 220)	0.349	23.5	14.72	198.5
	37	NiO(111)	0.533	15.62	22.17	450.45
	42.9	NiO(200)	0.176	48.26	7.17	47.22
	62.72	NiO(220)	0.36	25.74	13.45	165.9
NiO : Li 4%	31.88	LiNi ₂ O ₄ (220)	0.208	39.51	8.76	70.44
	33.54	Li ₂ NiO ₂ (100)	0.192	42.99	8.05	59.50
	36.88	NiO(111)	0.222	37.52	9.23	78.10
	43.4	NiO(200)	0.22	38.67	8.95	73.52
	49.38	(LiNi ₂ O ₂ 331)	0.1975	44.07	7.86	56.63
	62.92	NiO(220)	0.173	53.50	6.47	38.42
NiO:Li 6%	31.64	(LiNi ₂ O ₄ 220)	0.322	25.51	13.58	169.01
	33.46	(Li ₂ NiO ₂ 100)	0.252	32.75	10.57	102.55
	36.7	NiO(111)	0.44	18.92	18.30	307.05
	43.1	NiO(200)	0.48	17.70	19.56	350.73
	45.34	(LiNi ₂ O ₄ 400)	0.236	36.30	9.54	83.43
NiO:Li 8%	-----	-----	-----	-----	-----	-----

Fig.3. Pure Neo-Neuromuscular Morphology and Li-Stimulants were calculated by 0.02, 0.04, 0.06 and 0.08% Grammy, at 150 nm, showing the effect of doping on NiO and NiO:

Li film. The grain size corresponds to XRD test results. Table 2 shows granular size, surface roughness, and square root value of the mean roughness of all prepared films.

Table 2: AFM data for all prepared films

Sample	Grain size, (nm)	Roughness (nm)	Root mean square (nm)
NiO (Pure)	84.51	1.47	2.01
NiO:Li (2%)	74.17	2.61	3.1
NiO:Li (4%)	61.76	2.73	3.3
NiO:Li (6%)	74.32	2.43	2.84
NiO:Li (8%)	88.92	1.05	1.25



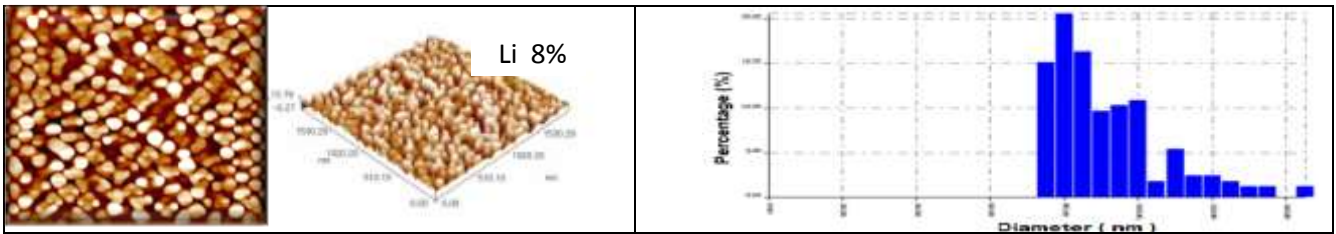


Fig.3:2 and 3D AFM images for all prepared films

Figure 4 shows the effect of wavelength (λ) on absorption in the spectral range 300-1100 nm for the NiO and Li-doped NiO thin films tested at 150 nm thickness. In the figure, we observe that the absorption edges turn to the longer wavelength (red shift), indicating that the value of the optical gap decreases with respect to increasing the concentration of Li. This is due to the presence of smuggled transitions in local states in the energy gap. The sharp absorption edge corresponding to the band gap emphasizes the good quality of the films grown.

The films show higher absorption of the shorter wavelength (UV) side and low absorption on the higher wavelength side (visibility). In the high wavelength, the photon does not have enough energy to interact with the atoms, so the photon will move, while in the low-wavelength region the incoming photons have enough energy to excite electrons from band equivalence to the connecting band, these photons are eventually absorbed within the material. The thickness is measured on 150 nm films .

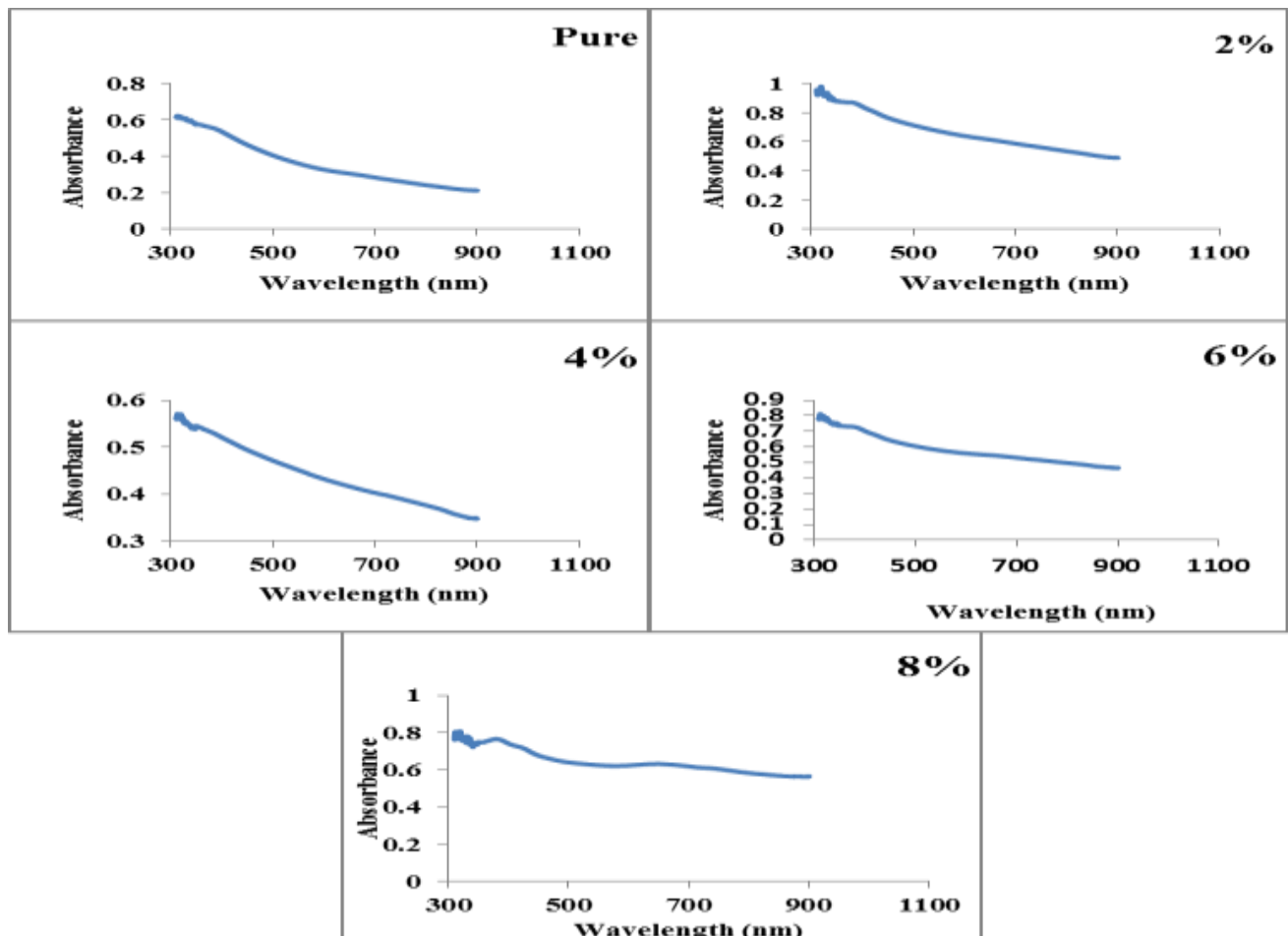


Fig. 4: Optical absorbance VS wavelength for all prepared films

Figure 5 shows the effect of wavelength (λ) on permeability at 300-1100 nm for NiO and Li-doped NiO films tested at 150 nm thickness. Neo-permeable membrane permeability can be used to 72% in visible areas and NIR for applications as window layers in solar cells.

Optical transmittance of samples prepared at different concentrations of me has a slightly low permeability, due to increased concentration of me. This behavior can be attributed to the structural properties of the gastric membranes, where photon scattering increases due to crystalline defects [12, 13].

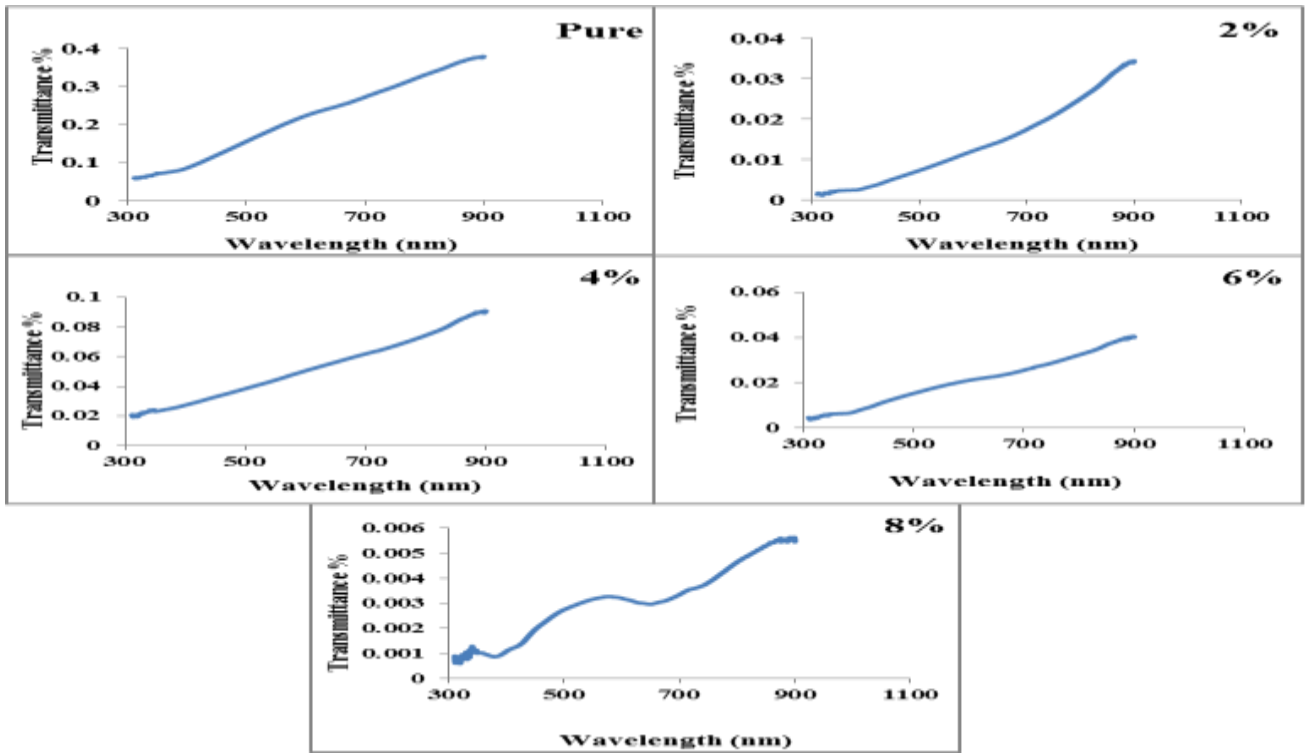


Fig. 5: Optical transmittance spectra VS wavelength for all prepared films

Figure 6 shows the wavelength effect on the optical absorption coefficient in the spectral range 300-1100 nm for the pure NiO and Li-doped NiO films examined at 150 nm thickness. We observe an increase in the values of the optical absorption coefficient

with increasing Li concentration, based on the fact that a small increase in absorption values was obtained when the dopant was increased. In the high absorption area, all films have $\alpha > 10^4 \text{ cm}^{-1}$ value, which increase the probability of direct transmission.

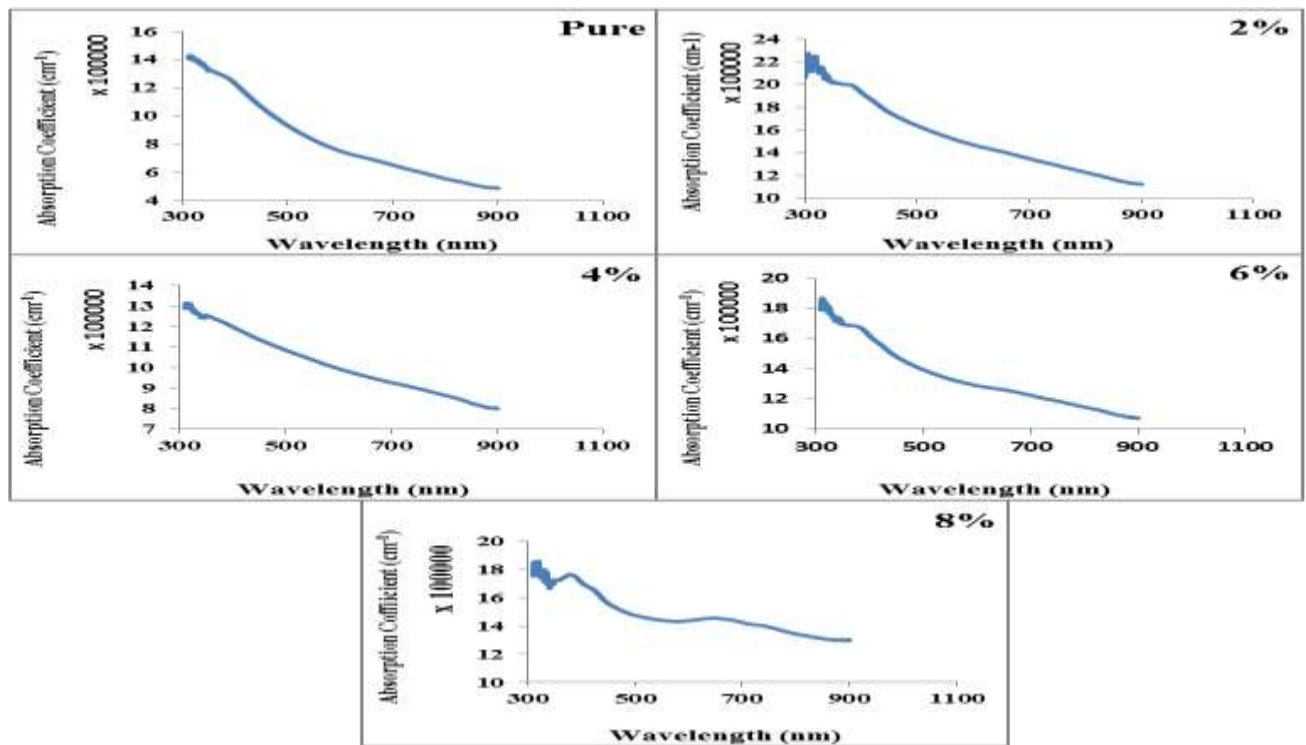


Fig. 6: The absorption coefficient for all prepared films

The optical energy gap of the intercept $(\alpha h\nu)^2$ VS can be obtained .Photon energy $h\nu$ for allowed direct transformations. The experimental values of $\alpha h\nu^2$ shown against NiO and LiO NiO contain 0.02, 0.04, 0.06 and

0.08 mol% of Li deposited at 300 ° C for 60 s and 150 nm thicknesses shown in Fig. 7.The value of the band gap energy from the straight line portion of the plot to the x-axis $(\alpha h\nu)^2 = 0$.

The linear nature of the soil on the absorption edge proves that all NiO and Li doping NiO films are semi-conductive with the straight band gap. The values of the optical energy gap, obtained by drawing the curves to $ah\nu^2 = 0$ for NiO and 0.02, 0.04, 0.06 and 0.08 mol) from Li doped NiO film were 2.4, 1.9, 1.6, 1.8, 2 eV respectively.

The reason for the change in the value of the energy of the optical band gap, with a concentration on the imbalance in the homogeneity and density of the translated cases, which increases by increasing the concentration of Li in the films deposited.

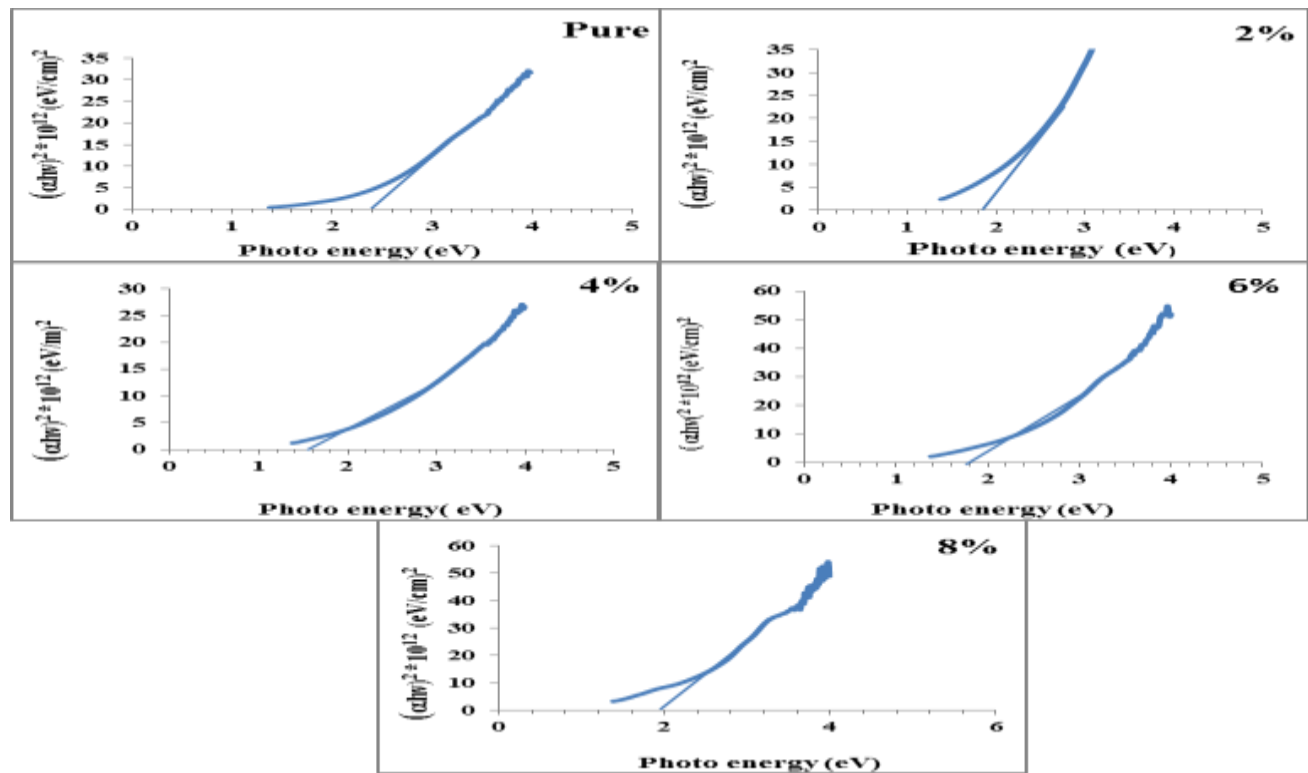


Fig. 7: Plot of $(ah\nu)^2$ VS. Photon energy ($h\nu$) for all prepared films

Conclusions

XRD results discovered that NiO and Li-doping was 0.02, 0.04, 0.06, and 0.08 thin film were found in polycrystalline and had a cubic structure. The XRD data showed the dominating peak is (111). (111)-Oriented NiO and Li: NiO films can be used as buffer layers that are deposited on oxide films with other orientations, such as c-axis oriented perovskite type ferromagnetic films and super conducting films. With the increase Li

concentration, the intensity of (111) peak was increased. The AFM results discovered that the surface of films is extremely smooth. With the Li content increase, and decreases in the roughness of film surface. The transmittance value of pure NiO film extends to 72% in the visible and NIR range, which is important for its applications as window layers in solar cells. The optical energy gap of NiO with concentration (0, 0.02, 0.04, 0.06, and 0.08) % of Li thin film was equivalent to 2.4, 1.9, 1.6, 1.8, and 2 eV.

References

1. IA Garduno, JC Alonso, M Bizarro, R Ortega, L Rodriguez-Fernandez, A Ortiz (2010) "Optical and electrical properties of lithium doped nickel oxide films deposited by spray pyrolysis onto alumina substrates" *Jour. of Crystal Growth*, 312: 3276-3281.
2. BT Rauta, SG Pawar, MA Chougule, Shashwati Senb VB Patil (2011) "New process for synthesis of nickel oxide thin films and their characterization" *Jour. of Alloys and Compounds*, 509: 90659070.
3. Y Sirotn, M Shaskolskaya (1982) "Fundamentals of Crystal Physics" (Mir Publishers, Moscow).
4. Nano Science instruments, on the site "<http://www.nanoscience.com/education/AFM.html>".
5. Ortega M, Santana G, Acevedo AM (1999) *Superficies Vacio*, 9: 294-295.

6. SM Sze, Kwok K Ng (2007) "Physics of Semiconductor Devices", 3rd, Ed. John Wiley & Sons, New York.
7. Hao-Long Chena, Yang-Ming Lu, Weng-Sing Hwang (2005) "Characterization of sputtered NiO thin films", *Surface & Coatings Technology*, 198: 138-142.
8. PS Patil, LD Kadam (2002) *Appl. Surf. Sci.*, 199: 211-221.
9. J Yang, DQ Shi, C Park, KJ, Song, RK Ko, HZ Lin, HW Gu (2004) *Physics*, 412-414 844,
10. HW Ryu, GP Choi, WS Lee, JS Park (2004) *J. Mater. Sci. Lett.*, 39.
11. HL Chen, YM Lu, WS Hwang (2005) *Surf. Coat. Technol.*, 198: 138.
12. Wen Guo, KN Hui, KS Hui (2013) "High conductivity nickel oxide thin films by a facile sol-gel method" *Journal of Materials Letters*, 92: 291-295.
13. Joseph DP, Saravanan M, Muthuraaman B, Renugambal P, Sambasivam S, Raja SP, et al (2008) "Spray deposition and characterization of nanostructured Li-doped NiO thin films for application in dye-sensitized solar cells". *Nanotechnology*.19: 485-707.