STRUCTURAL AND OPTICAL PROPERTIES OF N_2 DOPED ZnO THIN FILMS

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ABSTRACT: *ZnO thin films have a wide range of applications due to their wide band gap and easy doping. We report on the doping with nitrogen with different inflow rates in ZnO thin films in order to check the effect on optical transparency. These films are RF magnetron sputtered-deposited onto glass substrates and are characterized with the use of XRD and Spectroscopic Ellipsometer.*

Keywords: ZnO thin films, RF magnetron sputtering, Ellipsometer, doping and TCO

1. INTRODUCTION:

ZnO (zinc oxide) is a versatile material having a broad spectrum of potential application in the field of science and technology such as optoelectronics, photovoltaics, transparent conductive oxides, MEMS and NEMS [1]. These applications occur due to the presence of wide band gap of 3.37 eV [2]. ZnO has been extensively studied in doped form using Li, Na, and Cu, showing ease of doping, low cost and non-toxicity [3].

ZnO is supposed to be a good alternate for Indium Tin Oxide (ITO) thin films among all other transparent conductive oxides due to its low cost and high abundance [4]. The substitution of different dopants contributes to increase in the transparency and minimization in the resistivity of ZnO thin films [5-7]. ZnO intrinsically is n-type semiconductor because of Zn interstitials and / or oxygen vacancies.

N_2 is supposed to the best candidate for doping because the ionic radii of N_2 and Zn are similar which cause to lower the lattice imperfections (defects and vacancy formation) and strain in thin films. Moreover, N_2 is supposed to be non-toxic, easily available and low-cost dopant [1, 3].

Different depositions techniques are being used to deposit ZnO thin films. Sol-gel, Pulsed laser deposition, Molecular beam epitaxy, chemical vapor deposition, spin coating and RF magnetron sputtering [13] are some to be mentioned. Amongst all of these, RF magnetron sputtering is very reliable because it gives easy and precise control on doping concentration with extra pure and impurity free thin films as compared to other techniques [14]. In the present work we have deposited nitrogen-doped ZnO thin films by RF magnetron sputtering system at room temperature.**2.**

EXPERIMENTAL DETAILS:

N_2-doped ZnO thin films were deposited onto glass substrate by means of RF magnetron sputtering system. A 3" diameter target of ZnO (99.99% pure) is placed at 72mm distance with substrate. Three glass substrates firstly washed with detergent then 15 to 20 mins ultrasonically washed with acetone and IPA and then nitrogen dried were used.

High vacuum was attained by means of a turbo-molecular pump. The nitrogen inflow was fixed at 0, 5, 10, 15, 20, 25 and 50 sccm. The flow of Ar remained fixed at 50 sccm. Each sample had 30 mins of deposition time. The thickness of ZnO thin films varied (~ 300-500 nm) with different doping concentrations.

The crystal structure of thin films was obtained by X-ray diffractometer, PANalytical X'pert pro using CuKα radiation in the 2θ range of 20-80˚. Optical properties were studied by using J.A. Woolam's M2000 Spectroscopic Ellipsometer.

3. RESULTS AND DISCUSSIONS:

3.1. Structural Properties

The XRD pattern in Fig. 1 shows the pattern of N-doped ZnO thin films. The XRD pattern confirmed that the dominant peaks are those of ZnO with (002), (100), (101) and (103) hkl value.

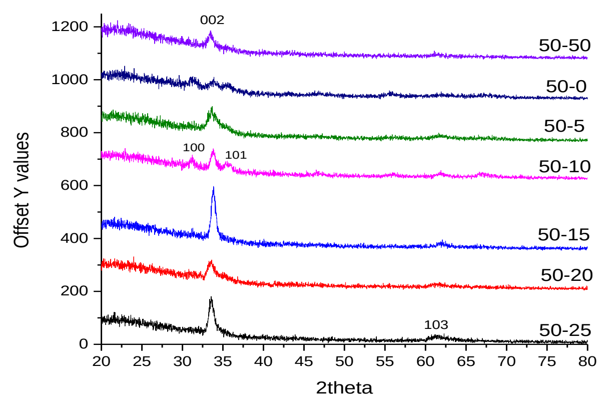
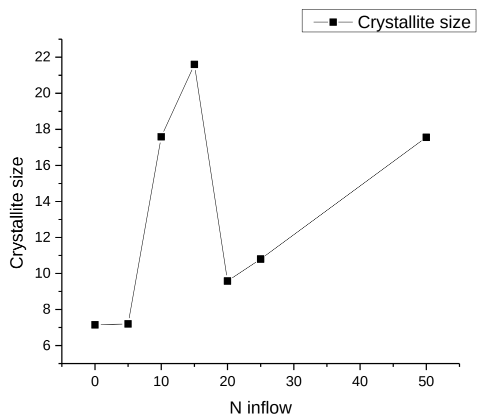


Fig. 1: XRD graphs of ZnO thin films

The XRD pattern of ZnO thin films shows a strong peak on (002) but the intensity of this and other peaks varies as N inflow varies. It can be clearly seen that the peak intensity with 15 and 25 sccm N_2 inflow rate recorded high peaks as compared to other samples. The shift is also seen in this peak from low 2θ towards high 2θ value, which contributes towards less crystallinity and tensile stress in the films with increase in N_2-inflow. Peaks of (100) and (101) disappeared with increase in N_2-inflow. This indicates that the material goes towards amorphous phase from strong crystal structure phase. The d-spacing, 2θ values and FWHM of each sample are summarized in the following table.

Table 1: Lattice parameters, FWHM, crystallite size and dislocation density of N_2 doped ZnO

N_2-inflow (Sccm)	2θ˚	a(Å)	c(Å)	FWHM (˚)	Crystallite size (nm)	Dislocation density (nm)
0	33.632	3.312	5.2337	0.090	7.15	0.01956
5	33.490	3.21	5.35	0.090	7.2	0.01929
10	33.832	3.26	5.298	0.472	17.58	0.00324
15	33.828	3.216	5.294	0.384	21.6	0.00214
20	33.224	3.23	5.388	0.864	9.58	0.0109
25	33.520	3.24	5.343	0.768	10.8	0.00857
50	33.437	3.237	5.358	0.472	17.56	0.00324



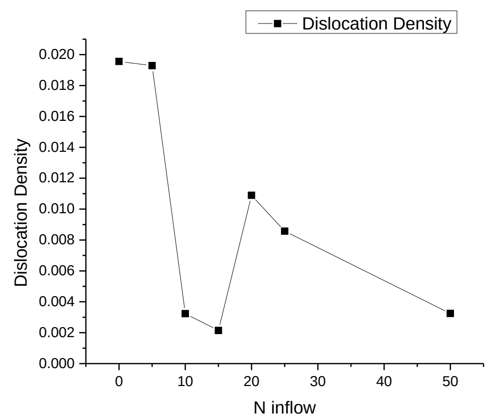


Fig. 2: (Left) Crystallite size variation with N_2 inflow; (Right) Dislocation density variation with N_2 inflow

The crystallite size of ZnO thin film was calculated by the well-known Scherrer formula:

$$D = \frac{0.9\,\lambda}{\beta \cos\theta} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots 1$$

In this equation the constant 0.9 is known as the proportionality constant and β denotes FWHM which is measured in radians and θ is the peak position [2, 7].

The Crystallite size of ZnO thin films increases with the increase of nitrogen inflow rate up to 15 sccm. The crystallite size is observed maximum and after that it decreased suddenly and then increased gradually showing a linear behavior.

Dislocation density can be calculated by the given formula:

$$\delta = \frac{1}{D2} \quad \ldots\ldots\ldots\ldots\ldots\ldots 2$$

The dislocation density is maximum at lower N_2 inflow and it decreases with the increase of N_2 inflow as shown perviously [6].

3.2. Optical Properties

The transmittance spectra of N_2 doped ZnO thin films were recorded using spectroscopic ellipsometer and are shown in Fig. 3. It can be seen that the maximum transmittance is in the wavelength range of 600-700 nm. Whilst, the highest transmittance is found for the N_2 concentration of 20 sccm, which is 97%. The average transmittance is found to be increasing with the increasing concentration of N_2 inflow.

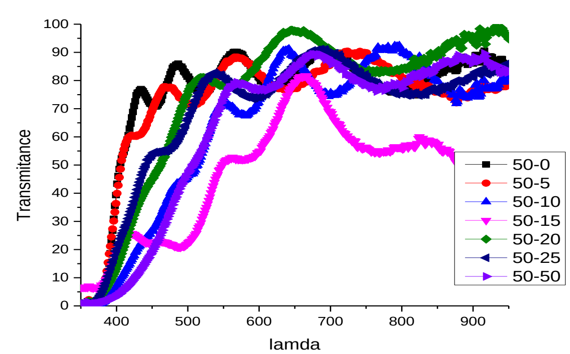


Fig. 3: Transmission vs wavelength graph of ZnO thin films with different N inflow ratio.

4. CONCLUSIONS:

We found maximum optical transparency of 97% when ZnO thin films were doped with 20sccm inflow ratio of Nitrogen respectively. These films were RF magnetron sputter-deposited onto glass substrates and were characterized through XRD pattern. The crystallinity of ZnO thin films decreased with the increase of N_2 inflow rates, which shows that the presence of N_2 leads ZnO thin films towards the amorphous behavior.

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