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Research Article

X-RAY PEAK PROFILE ANALYSIS OF $Zn_{1-x}Mg_xO$ THIN FILMS BY SILAR METHOD

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ABSTRACT

In this paper, we reported $Zn_{1-x}Mg_xO$ thin films were prepared by successive ionic layer adsorption and reaction (SILAR) method. The prepared films were characterized by x-ray diffraction. The hexagonal wurzite nature of the prepared material was confirmed. The micro-structural properties such as grain size, dislocation density, texture coefficient and structural properties such as lattice constants, bond length and bond angles were evaluated.

INTRODUCTION

Zinc oxide (ZnO) has been successfully included in the photonics, optoelectronics, spintronics, and gas sensors applications [1–3]. Zinc oxide (ZnO), a wide band gap (3.37 eV) and a large excition binding energy of 60 meV semiconductor, has attracted much attention for possible applications in optoelectronic devices [4–6]. The properties of ZnO nanostrucutres have changed considerably by doping metal in Zn lattice such as Fe, Al, Mn, Cr, Cu, Na [7-12]. Especially, ZnO can be alloyed with another high optical band gap II–VI compounds like magnesium oxide (MgO) to increase its band gap. ZnO:Mg is a semiconductor composed of two materials, zinc oxide and magnesium oxide, which can be easily controlled over a wide range of temperatures because the ionic radii of Mg^{2+} and Zn^{2+} are similar [13]. Improvements in ZnO:Mg dopant technology [14] have led to many new applications in electronics and optoelectronics [15].

Mg-doped ZnO thin films have been prepared using various methods, such as spray pyrolysis [16], pulsed laser deposition [17], chemical vapor deposition [18], radio frequency (rf) magnetron sputtering [19,20], electro-deposition [21], SILAR method [22], the sol–gel method technique [23]. It is also experimentally established that the structural and optical properties of these thin films are very sensitive to the deposition conditions [24]. Among these methods, the sol–gel method is an attractive one due to its simplicity and reproducibility. In the present study, $Zn_{1-x}Mg_xO$ thin films are prepared by SILAR method with different Mg doping concentration. The micro-structural properties such as grain size, strain and structural properties such as lattice constants, bond length and bond angles are examined by X-ray peak profile.

Experimental details

Materials

The chemicals used in this process are zinc sulphate, magnesium sulphate and sodium hydroxide. Deionised water is used throughout the process. The chemicals are purchased from merk India and used as received without further purifications.

Synthesis of $Zn_{1-x}Mg_xO$ nanostructure

$Zn_{1-x}Mg_xO$ thin films were prepared by using a dip coating (SILAR) technique. The precursor solution comprising 0.1 M

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Zinc Sulphate (99% emerk), 0.2 M sodium hydroxide with a pH value of 9±0.2 deposited at bath temperature of 90°C under optimized condition for pristine ZnO thin films. Before deposition, the glass substrates were cleaned by chromic acid followed by cleaning with acetone. The well-cleaned substrates were immersed in the chemical bath for a known standardized time followed by immersion in hot water for the same time for hydrogenation. The process of solution dip (step 1) followed by hot water dipping (step 2) is repeated for known number of times. The cleaned substrate was alternatively dipped for a predetermined period in sodium zincate bath and water bath kept at room temperature and near boiling point, respectively. According to the following equation, the complex layer deposited on the substrate during the dipping in a sodium zincate bath will be decomposed to ZnO due to dipping in hot water. The proposed reaction mechanism is according to the following equations

$ZnSO_4 + 2\ NaOH \rightarrow Na_2ZnO_2 + H_2SO_4\uparrow$
$Na_2ZnO_2 + H_2O \rightarrow ZnO + 2\ NaOH$

Part of the ZnO had so formed was deposited onto the substrate as a strongly adherent film and the remainder formed as a precipitate. For Mg doped ZnO films, suitable amount of $MgSO_4$ are added. The proposed reaction mechanism for the formation of Mg doped ZnO thin films is according to the following equations.

$Mn\ (SO_4.H_2O) \rightarrow Mn^{2+} + SO_4^{2-}$
$Zn\ (SO_4.7H_2O) \rightarrow Zn^{2+} + SO_4^{2-}$
$Na\ OH \rightarrow Na^{+} + OH$

The formation of Mg doped ZnO Thin films process could be expressed as
$Mn\ (SO_4.H_2O) + Zn\ (SO_4.7H_2O) + NaOH \rightarrow Mg\ ZnO + 2NaSO4 + H_2O$.

Characterization method

The prepared thin films are characterized by X-ray diffractometer (Model: XPERT-PRO) at room temperature. The wavelength of Cu-Kα line used in XRD is 1.54060 Å.

RESULTS AND DISCUSSIONS

The XRD pattern of $Zn_{1-x}Mg_xO$ thin films are shown in figure 1. The observed pattern indicates the prepared material has a hexagonal wurtzite phase of ZnO (JCPDS card no:89-7102). As the Mg level increases, the intensity of (002) plane decreases. Undoped and doped ZnO nanorods show the maximum intensity corresponding to the miller indices (002) [25]. This is the direct evidence that nanorods can be formed by the SILAR method simply by varying number of dipping.

Debye-Scherrer's method & Uniform deformation model

The crystallite size of the various doping levels of Mg doped ZnO samples are calculated from Debye-Scherrer's formula. Let λ be the wavelength of X-rays used and βhkl and θ are full width at half maximum and Bragg's angle corresponding to the maximum intensity peak. The Debye-Scherrer's (DS) formula is given as,

$$D = \frac{K\,\lambda}{\beta_{hkl}\,cos\theta}$$

The observed grain size for pure ZnO is 42.27 nm and Mg doped ZnO is ranges for 12.14 nm, 16.35 nm and 16.29 nm, for 0.05, 0.10 and 0.15 of Mg doping level respectively. According to uniform deformation model, we consider the prepared material is isotopic in nature and the strain is assumed to be uniform in all crystallographic direction. The Williamson-Hall equation according to UDM is given by [26]

$$\beta_{hkl}\cos\theta_{hkl} = \frac{K\lambda}{D} + 4\varepsilon\ \sin\theta_{hkl}$$

The values of $4\sin\theta_{hkl}$ is taken along the x-axis and $\beta_{hkl}\cos\theta_{hkl}$ is taken along the y-axis. The obtained plot is a strain line and form the intercept along y-axis, the grain size is calculated. The obtained grain size from UDM is highly coincidence with the result obtained from DS equation. The obtained results for crystallite size are shown in figure 2. High grain size is obtained for pure ZnO sample. The crystallite size decreases for Mg doped ZnO thin films.

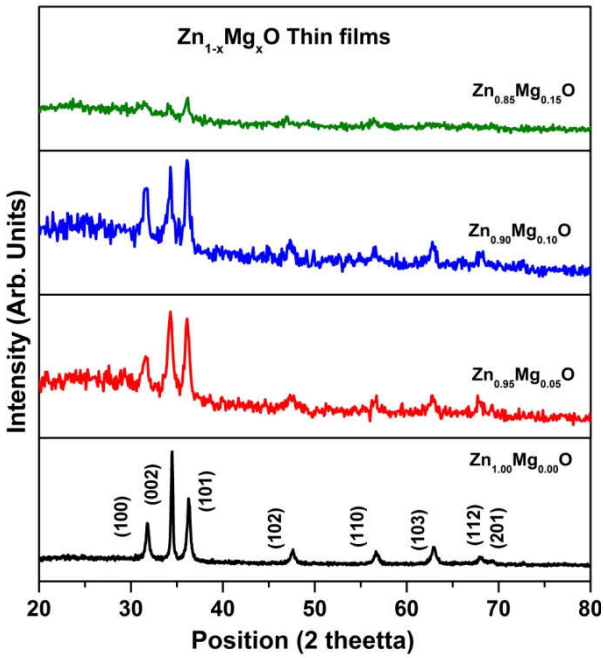

Fig 1 XRD Pattern of (a) $Zn_{1.00}Mg_{0.00}O$, (b) $Zn_{0.95}Mg_{0.05}O$, (c) $Zn_{0.90}Mg_{010}O$ and (d) $Zn_{0.85}Mg_{0.15}O$

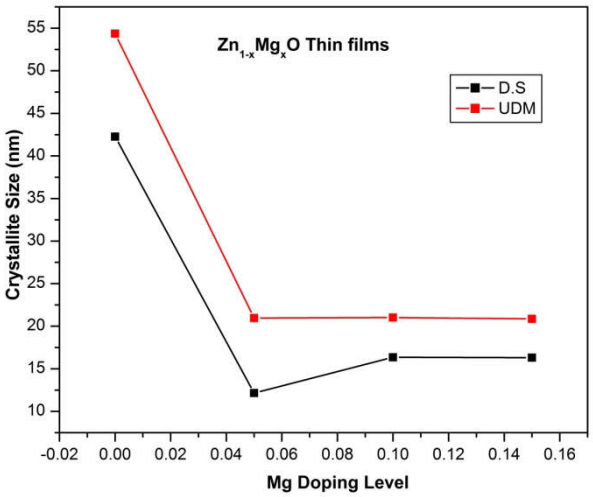

Fig 2 Crystallite size of (a) $Zn_{1.00}Mg_{0.00}O$, (b) $Zn_{0.95}Mg_{0.05}O$, (c) Zn0.90Mg010O and (d) $Zn_{0.85}Mg_{0.15}O$

Estimation of strain

According to Wilson method, the maximum strain ε_{hkl} is calculated by the d-spacing. Let d_0 is the standard d-spacing and Δd is the difference in the d-spacing between the observed value with standard value. The expression for strain is given below.

$$\varepsilon_{hkl} = \frac{\Delta d}{d_0}$$

The calculated strain for pristine ZnO is 2.434 x 10^{-3} and 6.029 x 10^{-3}, 6.004 x 10^{-3} and 6.029 x 10^{-3} for 0.05, 0.10 and 0.15 of $Zn_{1-x}Mg_xO$ thin films respectively. The results obtained, the strain of pristine doped ZnO nanostructure is highly greater than the Mg doped ZnO.

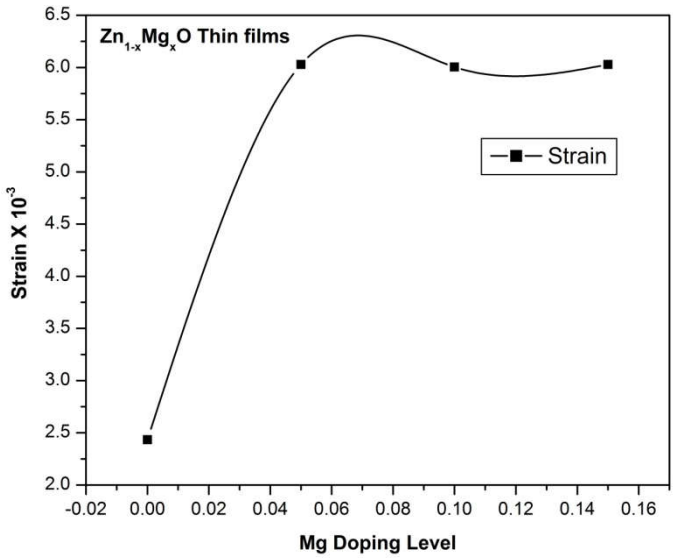

Fig 3 Strain

Unit cell analysis

The lattice constants 'a' and 'c' and hence the bong length and bond angles are evaluated.

$$\frac{1}{d^2} = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2}$$

Where d is the inter-planar spacing, 'a' and 'c' are lattice constants and h, k and l indicate the miller indices. The true lattice constants are evaluated using Nelson-Riley function (NRF) as given in the reference 25. The bond length is calculated as

$$L = \sqrt{\frac{1}{3}a^2 + (0.5 - u)^2 c^2}$$

Where u is 0.25+{0.33a^2/c^2}. The bond angles are given as

$$\alpha = \frac{\pi}{2} + \arccos\left[\left(\sqrt{1 + 3(c/a)^2\,(0.5-u)^2}\right)^{-1}\right]$$

$$\beta = 2arcsin\left[\left(\sqrt{\frac{4}{3} + 4(c/a)^2\,(0.5-u)^2}\right)^{-1}\right]$$

The obtained lattice constants, bond length and the bond angles are highly coincidence with the standard results.

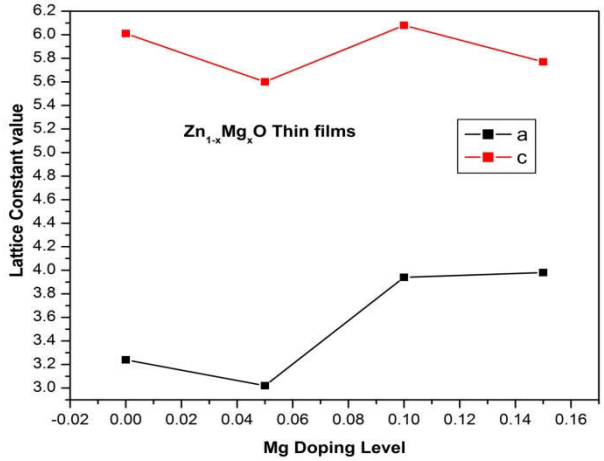

Fig 4 Lattice constants

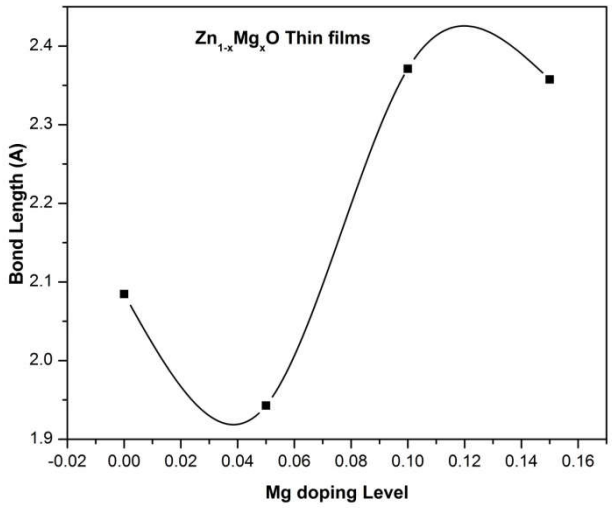

Fig 5 Bond Angle

Table 1 Micro-Structural and Structural Properties

Micro-Structural and Structural Properties	$Zn_{1.00}Mg_{0.00}O$	$Zn_{0.95}Mg_{0.05}O$	$Zn_{0.90}Mg_{0.10}O$	$Zn_{0.85}Mg_{0.15}O$
Crystallite size from DS equation (nm)	42.27	12.14	16.35	16.29
Crystallite size from UDM (nm)	54.35	20.95	21.02	20.85
Dislocation density	5.597 x 10^{14}	6.787 x 10^{15}	3.739 x 10^{15}	3.764 x 10^{15}
Strain x 10^{-3}	2.434	6.029	6.004	6.029
T.C	1.684	2.459	1.361	2.459
NRF	4.892	4.920	4.658	4.662
Lattice constant a (Å)	3.24	3.02	3.94	3.98
Lattice constant c (Å)	6.01	5.60	6.08	5.77
Bond length (Å)	2.0847	1.9429	2.3711	2.3576
Bond angle α(°)	116.19	116.17	106.38	102.92
Bond angle β(°)	101.98	102.00	112.37	115.14

CONCLUSION

$Zn_{1-x}Mg_xO$ thin films were prepared by Successive ionic layer adsorption and reaction method by varying the Mg doping concentration, such as (Mg=0, 0.05, 0.10 and 0.15). Crystallite size, strain, texture coefficient, lattice constants, bond angles are calculated from the X-ray peak profile analysis. The obtained results may trigger more work in this field.

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