Optik 125 (2014) 5776–5779

Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.de/ijleo

Correlation in calculations of electrical conductivity with and without undoped in Al, Co and In doped ZnO thin film

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ARTICLE INFO

Article history:
Received 17 October 2013
Accepted 29 May 2014

Keywords:
ZnO thin films
Semiconductor doping
Electrical conductivity
Crystallite size
Correlation

ABSTRACT

The transparent conductive pure and doped zinc oxide thin films with aluminum, cobalt and indium were deposited by ultrasonic spray technique on glass substrate at 350 °C. This paper is to present a new approach to the description of correlation between electrical conductivity and crystallite size with dopant concentration of Al, Co and In. The correlation between electrical and structural properties with dopant concentration suggests that the electrical conductivity of the films is predominantly estimated by the crystallite size and the concentration of Al, Co and In. The measurement in the electrical conductivity of doped films with correlation is equal to the experimental value of without undoped ZnO thin films, here the error is limited to zero %. The minimum error value was estimated in the cobalt and indium doped ZnO thin films. The correlation between the electrical conductivity and the crystallite size with the doping concentration was investigated.

1. Introduction

Zinc oxide (ZnO), being a wide band-gap (3.37 eV at room temperature) II–VI compound semiconductor [1,2], which is already used in various practical applications, such as optoelectronics [3], light emitting diodes [4], thin film [5], antireflection coatings, transparent electrodes in solar cells [6], gas sensors, surface acoustic wave devices [7], Schottky diodes and heat mirrors [8]. ZnO has been proposed to be a more promising UV emitting phosphor than GaN because of its larger exciton binding energy (60 meV) [9]. The resistivity values of ZnO films may be adjusted between 10^{-3} Ω cm and 10^{-4} Ω cm by changing the annealing conditions and doping [10].

The aim of this paper is study the possibility of the correlation between the optical and electrical properties of ZnO thin films with precursor molarity and doping level. Wojtczak et al. [11] presented a new approach to the description of the density of states for thin films which allows us to take into account the broadening of spectral lines, were the first to conclude that the formulation of the CPA approximation for thin films allows us to include the boundary conditions in the natural way and consider them without any additional approximations; secondary investigation is descript for the same boundary conditions given by various crystallographic orientations of the copper surfaces the Friedel oscillations of the electronic density appear. Tudose et al. [12] they studied the correlation of ZnO thin film surface properties with conductivity. There is a limited amount of literature dedicated to systematic and detailed studies on the surface evolution with growth parameters and their effect on the ZnO surface conductivity under reduction/oxidation. However, same works were investigated the dependence of physical properties of ZnO thin film as a function of parameters conditions such a temperature, thickness, oxidizing conditions, nitrogen addition and doping for characterizing the thin films [13–22].

In this paper, we have presented a new approach to calculate the electrical conductivity by the crystallite size, precursor molarity and doping level of doped ZnO thin film. Detailed calculations are developed from doped ZnO thin films with Al, Co and In.

2. Methods and model

The ZnO, ZnO:Al, ZnO:Co and ZnO:In samples were deposited on glass substrates by ultrasonic spray technique at a temperature of 350 °C with 2 min of deposition time. The crystallite size and electrical conductivity of the films were measured with doping level in the our papers, there we have studied the effect of various parameters such as doping level, growth times, substrate temperature, annealing temperature of the ZnO thin films [23–28] (see Table 1).

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http://dx.doi.org/10.1016/j.ijleo.2014.07.015
0030-4026/

Table 1
The electrical conductivity and crystallite size of ZnO, ZnO:Al, ZnO:Co and ZnO:In as a function of doping level [23–28].

Doping wt.%	ZnO:Al		ZnO:Co		ZnO:In	
	σ_e $(\Omega\,cm)^{-1}$	G_e (nm)	σ_e $(\Omega\,cm)^{-1}$	G_e (nm)	σ_e $(\Omega\,cm)^{-1}$	G_e (nm)
0	7.65	63.99	7.65	63.99	7.65	63.99
1	8.30	17.35	6.65	35.25	–	–
2	10.90	18.93	7.63	55.46	6.19	41.60
3	15.20	32.05	5.78	40.19	7.54	45.78
4	15.10	16.02	–	–	7.82	32.00
5	15.20	14.46	–	–	–	–

σ_e and G_e: experimental values.

Table 2
The variation of Empirical constants estimated by Eq. (3) of ZnO:Al, ZnO:Co and ZnO:In in the calculation with and without undoped ZnO film.

Empirical	Best estimate values of constants for					
	With			Without		
Constants	ZnO:Co	ZnO:In	ZnO:Al	ZnO:Co	ZnO:In	ZnO:Al
d	−1.052	−0.492	0.804	−1.024	−0.634	−0.303
e	5.260	4.679	7.725	5.586	6.175	4.883
f	−7.097	−2.024	−2.337	−8.591	5.970	−1.635

Table 3
The correlate electrical conductivity of ZnO:Al, ZnO:Co and ZnO:In as a function of doping level.

Doping (wt.%)	ZnO:Al		ZnO:Co		ZnO:In	
	σ_c $(\Omega\,cm)^{-1}$	σ_c $(\Omega\,cm)^{-1}$	σ_c $(\Omega\,cm)^{-1}$	σ_c $(\Omega\,cm)^{-1}$	σ_c $(\Omega\,cm)^{-1}$	σ_c $(\Omega\,cm)^{-1}$
	With	Without	With	Without	With	Without
0	14.61	7.65	7.35	7.65	7.52	7.65
1	7.60	10.09	6.65	6.65	–	–
2	10.13	11.27	7.63	7.63	6.19	6.19
3	15.90	13.84	5.78	5.78	7.54	7.54
4	15.10	15.30	–	–	7.82	7.82
5	14.54	15.92	–	–	–	–

σ_c: correlate value.

The correlation between the electrical and structural properties was studied for the electrical conductivity (σ) as a function of the crystallite size (G), precursor molarity M and doping level X_0 of doped ZnO thin films. These parameters correlates were resulting from the following equation:

$$\begin{cases} \sigma_{(*)} = \dfrac{\sigma_{(e)}}{\sigma_{(e)\mathrm{Max}}} \\ G_{(*)} = \dfrac{G_{(e)}}{G_{(e)\mathrm{Max}}} \\ M_{(*)} = \dfrac{M_{(e)}}{M_{(e)\mathrm{Max}}} \\ X_{0(*)} = \dfrac{X_{0(e)}}{X_{0(e)\mathrm{Max}}} \end{cases} \quad (1)$$

where $\sigma_{(e)}$, $G_{(e)}$, $M_{(e)}$ and $X_{0(e)}$ are the experimental data; $\sigma_{(e)\mathrm{Max}}$, $G_{(e)\mathrm{Max}}$, $M_{(e)\mathrm{Max}}$ and $X_{0(e)\mathrm{Max}}$ are maximal experimental values and $\sigma_{(*)}$, $G_{(*)}$, $M_{(*)}$ and $X_{0(*)}$ are the first values have been consisted in the correlate relationships.

3. Results

We have estimated the relationships between the electrical conductivity and the crystallite size with the precursor molarity in ZnO thin films is expressed as the following empirical relationships:

$$\sigma_{(c)} = a \times G^{(b+(c/M_{(*)}))} \quad (2)$$

where $\sigma_{(c)}$ is the correlate electrical conductivity; a, b and c are empirical constants as $a \approx 0.96106$, $b \approx -2.6984$ and $c \approx 2.6288$.

In this case, we have studied the correlation with electrical conductivity of doped films. These letters were deposited for the precursor molarity equal to 0.1 M, to perform the correlation in this section the electrical conductivity was measured with undoped ZnO thin film. The electrical conductivity was estimated as a function of crystallite size and doping concentration, so that the 0 wt.% is relate in the estimation. It is more important to calculate the electrical conductivity and relative error. In this section the empirical parameters (see Eq. (2)) a, b and c are constants for doped films. We found the following relationships:

$$\sigma_{(c)} = \exp(d \times X_{0(*)} \times G_{(*)}) \times (0.96106 \times G_{(*)}^{(0.5876)}) \times (1 + X_{0(*)}^{e \times G_{(*)} + f \times X_{0(*)}}) \quad (3)$$

where d, e and f are parameters constants dependences of dopant element and doping level, $G_{(*)}$ and $X_{0(*)}$ are the crystallite size and doping level, respectively. These parameters are collected in Table 2 and estimated as a function of dopant element. Table 3 presents the correlate values.

In order to evaluate the correlation between electrical conductivity and crystallite size with doping concentration by dopant elements, in this part the conductivity measured without the undoped ZnO thin films. In the end we have compared the relative error in tow parts for good quality.

4. Discussion

As shown in Fig. 1a–c, significant correlation was found between the electrical conductivity and the crystallite size of the doped ZnO