Comparative Study of the Structural Properties for Thin and Thick ZnO Films Deposited on PPC Plastic Substrates

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Abstract ZnO films with various thicknesses (0.4, 0.6, 0.8, 1 and 1.3 μm) had been prepared on PPC plastic bases by using DC sputtering. XRD results showed that all the films displayed principally ZnO (002) peak at 2θ = 34.115°, 34.01, 34.16, 34.07 and 34.12° with FWHM of 0.41°, 0.34, 0.27, 0.21 and 0.36° respectively, which is coincide with wurtzite hexagonal phase, indicated that films were preferentially grown along c-axis. XRD results also showed that the lattice constant and the crystallite size for the deposited thin films became larger than those for the thick film 1.3 μm; while the stress and microstrain increased for the thick films.

Keywords: Thin Films; PPC Plastic; Physical properties; Structural Properties; Thick Films

1. Introduction

ZnO is belong to the 2nd and 6th groups of periodic table. ZnO has a good sensitivity in the UV area and high photoconductivity [1]. ZnO has many applications like conducting electrodes, SAV filters, gas sensors, LED, and laser diodes [2-5].

ZnO thin films was deposited using various methods like DC sputtering technique, RFMS, PLD, MOCVD, CSP and Sol-Gel, metalorganic vapor phase epitaxy on various inorganic bases such as quartz, silicon, glass, diamond, NaCl, and InP [6-16]. But, plastic own lightweight and small size in comparison with inorganic bases [17], and employed in various applications like resilient sensors and curved detector modes. Plastic bases tool up lighter, more resistant to injury, flexible, and strong devices [18]; these assign make them appropriate as remote control, and circuits camcorders [19]. The base materials, were Polycarbonate, Polyarylate, Polyesstersulfone, Polyimide, Polyethylene terephthalate, Teflon, poly(ethylene naphthalate), thermoplastic Perplex, Plexiglas, Polyethylene naphthalate, and cellulose triacetate. [20].

Poly Propylene Carbonate (PPC), that employed as a base for deposition ZnO thin films, this may turn on a novel method for the manufacture of cheap optical devices [20]. Residual stresses play a considerable part in mechanical achievement and reliability of thin films. The presence of large residual stresses results in film buckling or cracking, and even interface delamination like a exemplary telephone-
cord peeling [21, 22]. The film is in a stressed state due to a difference in thermal expansion coefficients 

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2. Experimental work

ZnO films were grown on PPC plastic bases after cleaning by DC sputtering unit. The sputtering

unit operated with a base pressure of about 5x10⁻⁵ Torr; target material have a diameter of about 76.2 mm. Distance between the target and bases was 7 cm.

PPC was subjected to clean procedure before deposition. The target was pre-sputtered for 20 min to take
off any pollution, from target surface. Thickness was evaluated employing surface optical system
Filmetric F20-VIS. Structural properties of films were studied by XRD. Fig.1 shows two deposited films,
at the left with dark brown colored is 1.3μm thickness and the other is the film with 0.8μm thickness.

3. Results and discussions

Figure 2 offers XRD styles of the deposited ZnO films. All the films offer principally ZnO (002) peak at 2θ = 34.115°, 34.01°, 34.16°, 34.07° and 34.12° with FWHM of 0.41°, 0.34°, 0.27°, 0.21° and 0.368° respectively, that agree with wurtzite hexagonal phase of ZnO. The figure also displays other less intense peaks assigned to the planes (102) and (110) respectively that emphasize the forming of polycrystalline ZnO. This result agrees well with Lee et al. [24].

The crystallite size is obtained via Scherrer’s formula [25]:

$$D = \frac{K \lambda}{β \cos θ}$$

where D is the crystallite size, K is the shape factor (usually taken as 0.9), λ is the wavelength of the X-ray radiation, β is the full width at half maximum (FWHM) of the peak, and θ is the Bragg angle.
where $B$ is the FWHM, $\lambda$ is the X-ray wavelength, $\theta$ is the Bragg diffraction angle [25]. The results indicate that $D$ increases with increasing film thickness from 0.4 - 1 mm, while it decreases for the thick film with 1.3 nm thickness as shown in fig 3. This means that the thin films have better crystal quality and larger $D$ than the thick ZnO film. Table 1 summarizes XRD data.
The stress ($\sigma$) was calculated by using Equation [26].

$$\sigma = -233 \times \frac{c_{\text{film}} - c_{\text{bulk}}}{c_{\text{bulk}}} \text{ (GPa)} \quad (2)$$

where $c_{\text{film}}$ is the lattice parameter of c axis, and $c_{\text{bulk}}$ is the lattice parameter of bulk. The numerical values of $c_{\text{film}}$ is calculated by equation 3 [26]:

$$n\lambda = 2d_{hkl} \sin \theta \quad (3)$$

where $d_{hkl}$ is lattice spacing is obtained from the equation [26]:

$$d_{hkl} = \frac{1}{\sqrt{\frac{4}{3}h^2 + \frac{i^2}{a^2} + \frac{k^2}{c^2}}} \quad (4)$$
where $a$ and $c$ are lattice constants. The calculated $c_{\text{film}}$ of ZnO film is 0.5204 nm it is close to the value from (JCDD) card data for ZnO $c_{\text{bulk}}$ 5.2066 Å.

Stress values is found with negative sign indicates that films are compressive stress.

The total stress consists of two components: one, is the intrinsic stress and the second is the extrinsic stress [27]. In this paper, thickness varies from 0.4 to 1 μm, thus, the total stress was prevailing intrinsic.

Since substrate used in this research is plastic and this material bears a certain temperature, for this, the high temperatures resulting from the long period of film evaporation for 1.3 μm, led to the curvature of the substrate, which caused high stress in the deposited film. For this reason, we believe that this film showed less structural properties quality compared to the other films, also, we can expect that the stress in our prepared thin films is intrinsic, while in the thick film it can be considered as an extrinsic because of the long deposition time and the plastic substrate as offer in Fig. (1).

Figure 4 offers the difference of stress with film thickness and Table 1 lists the variance of lattice parameters, $D_i$, $\sigma$, and $e_{zz}$ with the film thickness.

![Fig. 4 : the variation of stress with film thickness.](image)

The strain ($e_{zz}$) originates principally due to lattice mismatch between film and base can be calculated from the lattice constant $c$ value in the z-direction using the following equation [27]. Fig. 5 shows the strain against film thickness.

$$e_{zz} = \frac{c_o - c}{c_o} \times 100\% \quad (5)$$

All the films exhibit tensile strain and from Table 1, the compressive stress decreases with increasing film thickness from 0.4 to 1 μm, while the sample prepared with the thick thickness (1.3 μm) shows an increase in stress, this may be due to the low structural properties as shown from the XRD result.
The dislocation density was obtained from the equation 6 [28]:

$$\delta = \left( \frac{1}{D} \right)^2$$  \hspace{1cm} (6)

Figure 6 displays the dislocation density against films thickness. As mentioned before, the crystallite size increased gradually from 20.27 to 38.48 nm with the increase of thicknesses from 0.4 to 1 \(\mu\)m for the deposited thin films, while it decreased for the deposited thick film to be 12.15 nm. The larger D and smaller FMHM values mark to better crystallization. \(\delta\) decreases with increasing thicknesses for thin films, which may be due to a decrease in the content of lattice imperfections. [28].

Fig. 5: Strain as a function of film thickness.

Fig. 6: The dislocation density as a function of film thicknesses
From all the obtained results and from the data in Table 1, for the thin films, that strain ($\varepsilon_{zz}$) in the film is tensile, indicating the existence of more relaxed films for higher thickness as shown in Fig 5. As thickness increases, the amount of ZnO reaching base surface increases to form film and therefore electrostatic interaction between ZnO particles becomes larger thereby increasing the probability of more ZnO particles to be gathered together forming a grain. But after one micron, as it’s known that the film change to a thick film, we notice that the crystallite size decreases, this might be due to heat generated by the sputtering process in the film of (1.3) micron which affected the order of crystallinity and increases the compression stress. Fig. 7 shows the comparison between the stress and strain in both the thin and thick deposited films as a function of thickness. These results are in agreement with Rao et al [27].

![Fig. 7: The stress and the strain of the intended films.](image)
4. Conclusion

This work was a trial to calculate and compared the stress and strain for thin and thick films, which was as the authors believe that it is achieved for the first time. It was noticed that the stress and strain decreased as the thickness of thin film increase, but for a thick film, the situation was reversed. It can be concluded that ZnO thin films deposited on PPC substrates had better crystalline structure than the thick one; these results maybe give a good improvement to use a thin film for many applications better than the thick one.

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