Thickness Influence on Structural and Optical Properties of ZnO Thin Films Prepared by Thermal Evaporation

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Abstract

Zinc Oxide transparent thin films (ZnO) with different thickness from (220 to 420)nm ±15nm were prepared by thermal evaporation technique onto glass substrates at 200 °C with the deposition rate of (10 ± 2) nm sec^{-1}, X-ray diffraction patterns confirm the proper phase formation of the material. The investigation of (XRD) indicates that the (ZnO) film is polycrystalline type of Hexagonal and the preferred orientation along (002) plane. The Optical properties of ZnO were determined through the optical transmission method using ultraviolet-visible spectrophotometer with wavelength (300 – 1100) nm. The optical band gap values of ZnO thin films were slightly increased from (2.9 - 3.1) eV as the film thickness increased.
Key words: thin films; structural properties; optical band gap.

Introduction

Zinc Oxide (ZnO) has a direct band gap semiconductor with 3.37 eV at room temperature.[1] polycrystalline ZnO has found numerous applications, such as transparent electrode in Solar Cells and flat panel displays as well as for the fabrication of grating in Optoelectronic devices, Window in antireflection coatings and Optical filters[2].

There are different methods available to prepare Zinc Oxide, such as pulsed laser deposition, chemical vapor deposition[3], etc. ZnO- based devices have attracted significant interest since they present sensitivity to various gases, high chemical stability for doping, non- toxicity and low cost[1]. Many of searchers works on ZnO thin films as [1-4]. The aim of The present work is to study the structural and optical properties of ZnO films which prepared by the thermal evaporation technique at different thickness.

Experiment

The metallic Zn films were deposited by thermal evaporation under vacuum onto clean glass substrates at different thickness (220, 320, 420)nm ± 15nm. A cylinder chamber of height 8 cm at top substrate vacuum system used was about 5.5×10^{-5} Torr. After preparation, the as – deposited Zn films were heated under air at flow rate 400 scuum at temperature 400 °C for two hours.

The film thickness was determined by ultrasound method. The crystalline structure of studied films was investigated by X-ray diffraction (XRD) analysis using Cu - K_α radiation (λ = 1.541 A°) in the range (2θ=20° – 80°).The films transmittance was measured using a UV – VIS spectrophotometer in the wavelength range(300 – 1100) nm.

Results and Discussion

Fig. (1) shows that (ZnO) films of different thicknesses are polycrystalline in nature with orientation along (002) plane. We see an increase in the intensity with the increase thickness material crystallization order will increase.

Fig. (2) shows the increase of peak intensity and decrease of the full width at half maxima (FWHM) as the thickness of ZnO film increase[3],where thickness increase make atoms packet as good and improve in structure this make (FWHM) decrease.

The crystallite size has been estimated from the FWHM of (002) diffraction peak by the scherrer relation [4]:

$$l = \frac{0.94\,\lambda}{\beta\, cos\theta} \;\ldots\ldots\ldots\ldots\ldots(1)$$

Where l is grain size, λ is the wavelength of X – ray radiation, θ is the Bragg angle of the (002) peak, β is the angular width of the (002) peak at a half of its maximum intensity (FWHM).

The mean crystallite dimensions calculated from Eq.(1), It is observed that the crystallite size reduces slightly for increased thickness films (19.8, 18.9, 17.7 nm).

The lattice parameters have been calculated using the relation [5]:

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

The d_{hkl} parameter was deduced from the XRD pattern. The values are found to be very much close to the standard values of hexagonal ZnO. In a real ZnO crystal the wurtzite structure deviates from the ideal arrangement by changing the c/a ratio or u parameter [6]. The c/a ratio and u parameter for the films deposited are computed and given in table (1). The lattice constants range from 3.253 to 3.258 for "a" parameter and from 5.215 to 5.220 for "c" parameter. The c/a ratio and u parameter vary from 1.603 to 1.602 and from 0.379 to 0.378 respectively.

All these films shows good optical transmittance (> 80 %)with wavelength (950 – 1100)nm in the visible and near – infrared range as shown in Fig.(3). Their high transmission in the visible range makes these films excellent candidates for transparent window materials in solar cells. The transmission of ZnO thin films decreased as the thickness increased because the atoms packed to gather as good.

This seems to came from the change in reflectance due to light interference of the zinc oxide thin film, similar behavior involving a decrease in the transmission of the film thickness increases has been reported in the literature[7, 8].

The optical band gap E_g was determined by analyzing the optical data with the expression for optical absorption coefficient α and the photon energy $h\vartheta$ where [9]:

$$\propto h\vartheta = K\,(h\vartheta - E_g\,)^{1/2} \;\ldots.(3)$$

Where h is the planck constant, ϑ is the frequency of the incident light. The optical band gap value (E_g) can be obtained by plotting $(\propto h\vartheta)^2$; $h\vartheta$ is the photon energy as shown in Fig. (4) As the film thickness increased from 220 nm to 420nm, the value of optical band gap gradually increased from (2.9, 3.0, 3.1) eV because of crystallization material increase , So position levels reduced near valance and conduction bands, that increased value of optical band gap , similar to other repots [3,4]. The low energy band gap could be attributed to defects and impurities[3].

Conclusion

ZnO thin films with various thicknesses were prepared on glass substrates by the thermal evaporation technique. The XRD patterns of the films showed good crystallinity. The optical bad gap values of ZnO thin films decreased as the film thickness increased. The optical properties that were observed for transmittance films of ZnO indicate that they may be used as window layers in solar cells.

References

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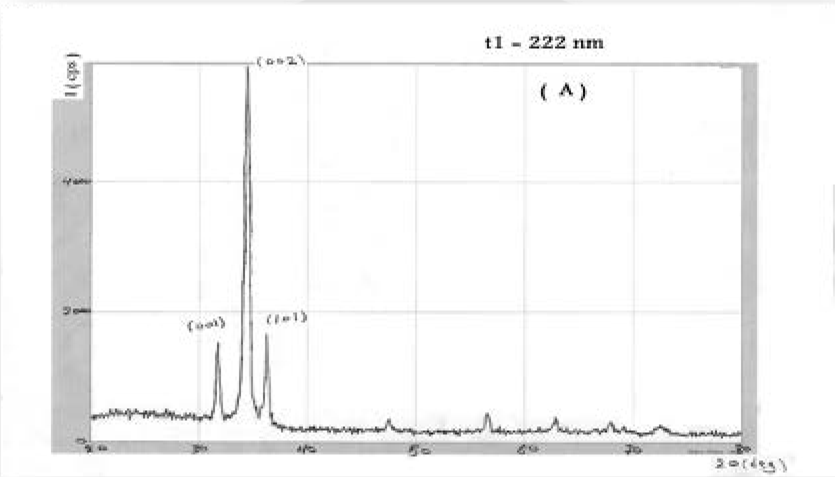
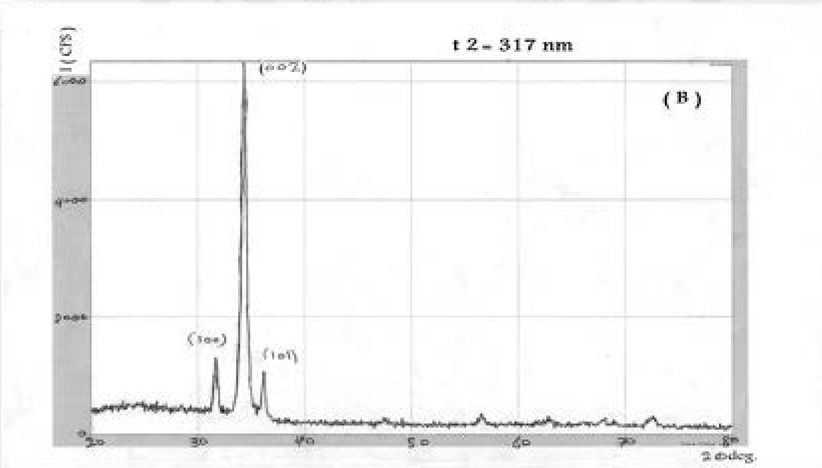
Table(1):Lattice parameters of ZnO films prepared by thermal evaporation.

Thickness t nm	(a) A°	(c) A°	c/a	$u=\frac{1}{3}\frac{a^2}{c^2}+\frac{1}{4}$ [5]	Ideal values c/a	Ideal values u
220	3.253	5.215	1.6030	0.3795	1.633	0.375
320	3.257	5.220	1.6025	0.3784		
420	3.258	5.220	1.6021	0.3785		





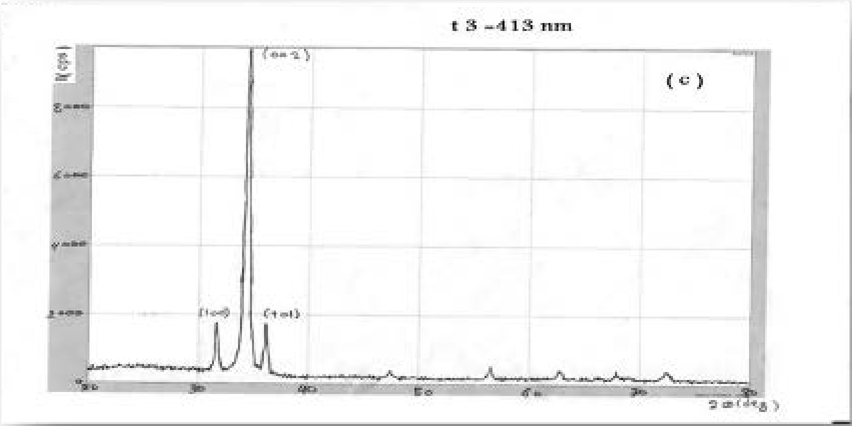


Fig. (1): XRD spectrum of ZnO films with different thickness (A) 222nm, (B) 317nm and (C) 413nm

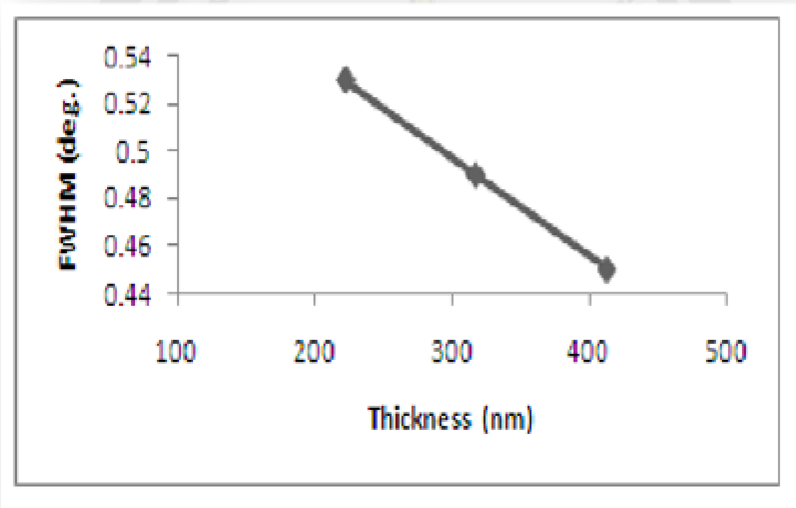


Fig.(2): Dependence of FWHM on the thickness of ZnO films.

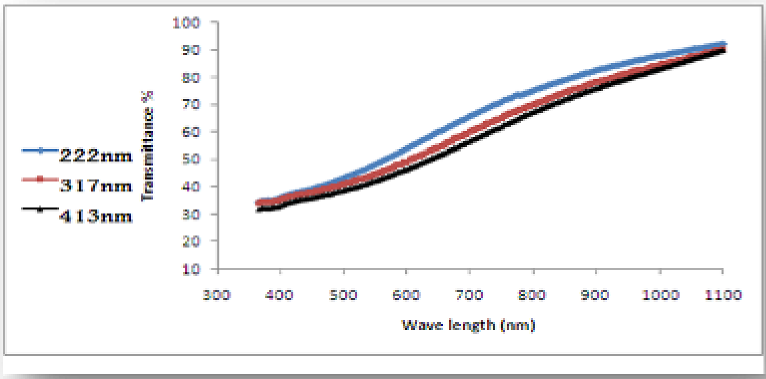


Fig.(3): Transmission as function of wavelength for ZnO films with different thicknesses

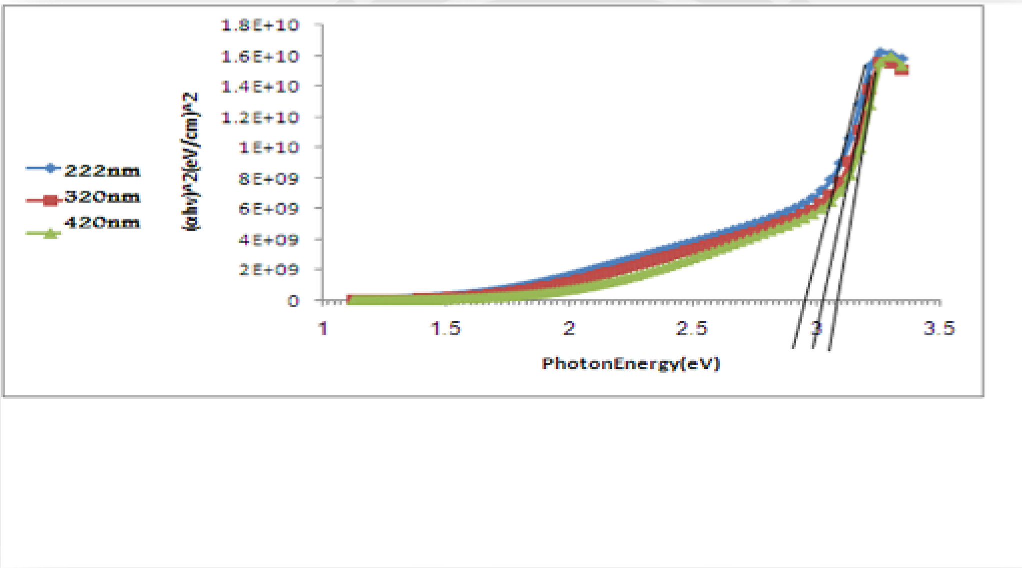


Fig. (4): A plot of $(\alpha h\nu)^2$ as function of photon energy for ZnO films with different thicknesses

تأثير السمك على الخواص التركيبية والبصرية للأغشية ZnO المحضرة بطريقة التبخير الحراري الفراغي

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الخلاصة

حضرت أغشية رقيقة لأوكسيد الخارصين ZnO بتقنية التبخير الحراري الفراغي على قواعد من الزجاج بدرجة حرارة أساس °C 200 وبمعدل ترسيب(10 ±2) $nm\ sec^{-1}$ لسمك مختلف من (220الى 420)nm ± 15nm، ان حيود الأشعة السينة بينت أن الأغشية ذو تركيب متعدد التبلور والاتجاه السائد هو للمستوي (002). حددت الخواص البصرية لأوكسيد الخارصين عن طريق النفاذية البصرية باستعمال مطياف Ultra Violet – Visible ضمن الاطوال الموجية nm(1100 -300) وكانت قيمة فجوة الطاقة البصرية للأغشية تتراوح بين eV(2.9) الى eV (3.1) بزيادة سمك الغشاء.

كلمات مفتاحية: الأغشية الرقيقة، الخصائص التركيبية، فجوة الطاقة البصرية.