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Effect of Annealing Temperature on the Structural and Optical Properties of The CdO Thin Films Prepared By Vacuum Evaporation Thermal Technique

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Abstract

Cadmium Oxide films have been prepared by vacuum evaporation technique on a glass substrate at room temperature. Structural and optical properties of the films are studied at different annealing temperatures (375 and 475) ˚C, for the thickness (450) nm at one hour. The crystal structure of the samples was studied by X- ray diffraction. The highest value of the absorbance is equal to (78%) in the wavelength (530) nm, at annealing temperature (375) ˚C**.** The value of at a rate of deposition is (10) nm/s. The value of optical energy gap found is equal to (2.22) eV.

Keywords*:* CdO thin films, X-ray diffraction, Structural, Optical proper ties, Absorbance, Bandgap

Introduction

Transparent conductive oxides (TCOs), an attractive type of semiconducting materials that are both optically transparent and electrically conductive, have potential application in optoelectronic devices such as solar cells, photovoltaic, flat panel displays, transparent electrodes, ohmic contact to LEDs, and heat reflectors [1–4]. In recent years CdO-based TCOs (binary semiconducting oxides, SnO_2, ZnO, In_2O_3, CdO, Ga_2O_3 etc, in thin films) received much attention due to their exceptional carrier mobility, nearly metallic conductivities and simple crystal structure [5]. Many techniques were adopted to grow CdO films such as: thermal evaporation [6], metal vapor organic deposition [7], spray pyrolysis [5], rapid photothermal oxidation of Cd [8], and pulsed laser deposition [9].

Cadmium oxide CdO is conducting, transparent in the visible region with a direct band gap of (2.5) eV and indirect band gap of (1.98) eV [10].The physics associated with these properties of nanocrystallites of II–VI semiconductors have been very interesting because of thinking the phenomena in a new point of view with the properties exhibited by them.[11]

Various techniques have been employed to prepare CdO thin films such as spray pyrolysis [12], rapid deposition technique [13], sol – gel spin coating [14]. In this paper CdO thin film was prepared by thermal evaporation technique. According to our knowledge, such work on CdO films obtained by thermal evaporation technique has not been reported. In this article we present characterization properties CdO films prepared by thermal evaporation method, such as the structural and optical properties. The influence of thicknesses on the film characteristic properties is investigated.

Experiments

The studied CdO thin films prepared by thermal vacuum technique at room temperature and annealing temperatures (375 and 475) ˚C, for the thickness (450) nm, we obtained the metal bulk Cd thin films (from Fluka A.G/Germany), were evaporated in vacuum, at room temperature, onto precleaned glass substrates, with (2.6 x 2) cm^2 area. The distance used between the substrate and the boat is (10) cm, and the thermal pressure is equal to (4.8 X 10^{-5})Torr. During Cd film heating, the color varied from silvergray at room temperature to black-brown at annealing temperatures (375 and 475) ˚C. After deposition, the obtained in the same conditions Cd thin films were divided in subjected to a gradual heating in air with the rate of (5) K/min. In order to get CdO material is prepared from oxidation of samples by the process of cadmium deposition in the thermal oven temperature (350) ˚C at one hour.

The Structural characterization of the films has been carried out using XPERTPRO X-ray diffractometer. (XRD--6000/7000,SHIMADZU CORPORATION). The incident radiation was Cu Kα filtered by Ni filter. The grain sizes of the film (g.s) were determined by the measured FWHM values of the strongest (111) reflection and estimated. The transition spectra of the films have been recorded using of the type (UV – VIS – Spectrophoto Meter UV - 1800).

Results and Discussion

Structural studies

The X-ray diffraction (XRD) patterns of the (CdO) films prepared at different annealing temperatures (375 and 475) ˚C, as shown in Figure.1. The presence of several peaks in the XRD patterns reveals that all the films are polycrystalline. The micrographs and corresponding diffraction pattern of CdO thin films for different annealing have been shown in Figure.1, From the diameter of the rings, which correspond to reflection from (111) and (222) planes of cubic CdO. For the CdO films, the main characteristic peaks are assigned to the (111), orientation at (2θ) angles, which are well matched with the standard data for the CdO crystal with rock salt cubic structure.[JCPDS data card No.050640]. Further it can also be seen that the lattice parameter (*a*) for the films works, which also matches very well with the standard value of (0.4695) nm [JCPDS data], as show in Table 1.

The relatively stronger intensity of the peak (111) indicates preferential orientation of the film and similar behavior has also been reported by other researchers [15]. From the XRD patterns it can be seen that as the temperatures increases the peak intensities increasing and it reaches a maximum at annealing, indicating an improvement in crystallinity up to (475) ˚C. This shows that a process annealing temperature of (475) ˚C is optimum for preparing CdO films by vacuum evaporation method. Such trend that the peak intensity increases up to certain process annealing temperature and then falls has been reported by several investigators who have studied CdO films grown by various techniques like thermal oxidation of evaporation [16]. This trend may be attributed to the variation in the amount of oxygen intake and energy of ad atoms. The mobility of ad atoms and clusters on the surface of substrate is proportional to their energy.[14]

Grain size value calculate is by the Scherrer formula.1, that the increasing in annealing temperature leads to an increase in the rate of grain size, as the evident in the (111) plane, and as in Table:1. This means an improvement in the structural properties of the film (nanocrystallin), because the display curved at the mid-intensity inversely proportional to grain size, as in equation 1.[15]

$$D = \frac{K\lambda}{\beta \cos\theta} \quad \ldots\ldots\ldots\ldots\ldots \quad (1)$$

where: D = Crystalline grain size (nm).

K = is a constant (0.94) of the CdO.

β β = FWHM of the observed peak (deg).

λ = wave length of the X-ray diffraction (nm).

Thus, the decrease FWHM leads to an increase in the size of particleboard. Note from the Table,1, that most of the values that are calculated responsive to this proportionality. Table: 1, lists the lattice constant (a) and grain size of (111) peak. From these results we can notice that the fundamental effect of vacuum evaporation is related to an increase in crystallites size and a decrease in the lattice constant. The growth process is affected by the following process; namely cold-worked annealed metal with flattened grains, will give essentially the same microstructure of worked and recrystallized grains, and be clear in the article type (Fcc), where is the CdO films of this type which is in agreement with previous results [15,17]

The Texture coefficient represents the texture of the particular plane [18], and is used to quantify the preferred orientation. For a preferential orientation the Texture coefficient should be greater than one. The Texture Coefficient (TC (hkl)) for the various planes at different annealing temp has been calculated using the relation:[19]

$$TC(hkl) = \frac{I(hkl)/I_o(hkl)}{1/N \sum I(hkl)/I_o(hkl)} \qquad \ldots\ldots\ldots\ldots(2)$$

where: $I(hkl)$ is the observed indensity of the (hkl) plane, I_o (hkl) is the standard intensity of the (hkl) plane, taken from the JCPDS data and N is number of diffraction peaks.

The results obtained for the films grown at (375, and 475) ˚C. It is seen that the TC is maximum for (111) plane for all the films deposited at different annealing. This shows that the (111) plane is the preferred orientation and that there is neither orientation change nor phase change with process temperature [20]. The values of some structural parameters determined for analyzed CdO samples are summarized in Table.1.

Table.1, one can see that the calculated values of TC(hkl) are deviated from unity, especially those corresponding to (111) and (222) planes. This indicates that the respective films have the largest preferred crystallographic orientation along the (111) diffraction plane. Such higher values for the texture coefficient have also reported by F.C. Eze for reactive vacuum evaporated CdO films deposited at various partial pressure of oxygen, [14 and 20]. So, one can conclude that in both cases (of CdO films obtained by thermal oxidation of vacuum evaporated Cd films and of those obtained by reactive vacuum evaporation) occur similar growth mechanism of the CdO crystallites.

Optical studies

The transmittance and absorbance spectra of spin coated CdO thin films prepared at annealing temperatures (375 and 475) ˚C. The optical transmission in the visible region of the CdO films increase with the annealing and attain a maximum values, as shown in Figure.2. Hence (375) ˚C may be considered at this stage the absorbance is (nearly 78%) in the wavelength (530) nm, from the relationship:[21]

$$A = 2 - \log T\% \qquad \ldots\ldots\ldots\ldots(3)$$

where: A, T are the absorbance, and transmittance, respectively.

The increase in visible transmittance of the film with annealing temperature up to (475) ˚C may be attributable to the improvement in the crystallinity of the crystallites and improvement in the structural and surface homogeneity of the films. The band gap which is of the material and exponent $(n)(n)$ depends on the type of transition. The calculated energy gap is for direct transition from the relationship:[21]

$$(\alpha h v)^{1/n} - A\left(hv - E_g\right) \quad \ldots\ldots\ldots\ldots(4)$$

where: A is constant, E_g E_g is the optical band gap energy, hv and α is the photon energy and absorption coefficient, respectively.

To determine the possible transitions $(\alpha h\nu)^{\frac{1}{n}}$ vs. $(h\nu)$ is plotted and corresponding band gap was obtained from extrapolating the straight portion of the graph on $(h\nu)$ axis. The direct band gap is calculated from $(\alpha h\nu)^2$ vs. $(h\nu)$ plots by the point [$(\alpha h\nu)^2$ = 0]. The direct band gap from $(\alpha h\nu)^2$ vs. $(h\nu)$ plots by the point [$(\alpha h\nu)^2$ = 0] lies in the range (2.22) eV. as shown in Figure. 3. The value of the energy gap for CdO films prepared at different annealing temperatures (375 and 475) ˚C for the films decrease from the value of (2.175) eV to the value of (2.1) eV.[22]

It is explains that so, there may be more than one interband absorptions for these nanocrystalline CdO samples. These might be due to the fact that for nanoparticles (size -few nm) as surface to volume ratio increases, so defect states increase due to increase of surface area and strain than that of bulk CdO. These defects create states at different energies in the band gap and there may be some finite transition probabilities from these states. Hence due to the absorption of energy by the defect states situated at different energies within the forbidden region (for our nanocrystalline CdO thin films), we get different linear segments in Figures.3.[11]

Conclusion

Thin films of Cadmium Oxide have been prepared by vacuum evaporation method. XRD shows the diffraction peaks characteristic to the CdO faces centered cubic (FCC), with lattice parameter (a = 0.469±0.004) nm, The average g.s of (111) orientation grains of the studied polycrystalline film annealed at (375 and 475) ˚C was found to Direct band gap energies were determined. The annealing temperature increases due to increase of transmittance which is deceasing absorption which of the value (nearly 78%) in the wavelength (530) nm, at annealing temperature (375) ˚C. The optical energy gap value of the range; (2.1 – 2.175) eV have been obtained that is decreasing bandgap where increased of annealing temp.

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Table (1): *T* – annealing temperature, D grain size, 2θ (111) - diffraction angle corresponding to (111) planes, a – lattice constant to (111) planes, TC (hkl) - texture coefficient for various planes

TC (hkl)			a 111 (nm)		2θ 111 (deg)		D 111 (nm)	(*T*) Annealing (°C)
(222)	(200)	(111)	XR-D	JCPDS	Experimental XR-D	Standard JCPDS		
1.04	-	0.96	0.4699	0.4695	33.150	33.001	47.47	R.T
1.23	0.18	1.59	0.4734	0.4695	32.706	33.001	49.91	375
1.25	0.31	1.25	0.4738	0.4695	32.710	33.001	51.1	475

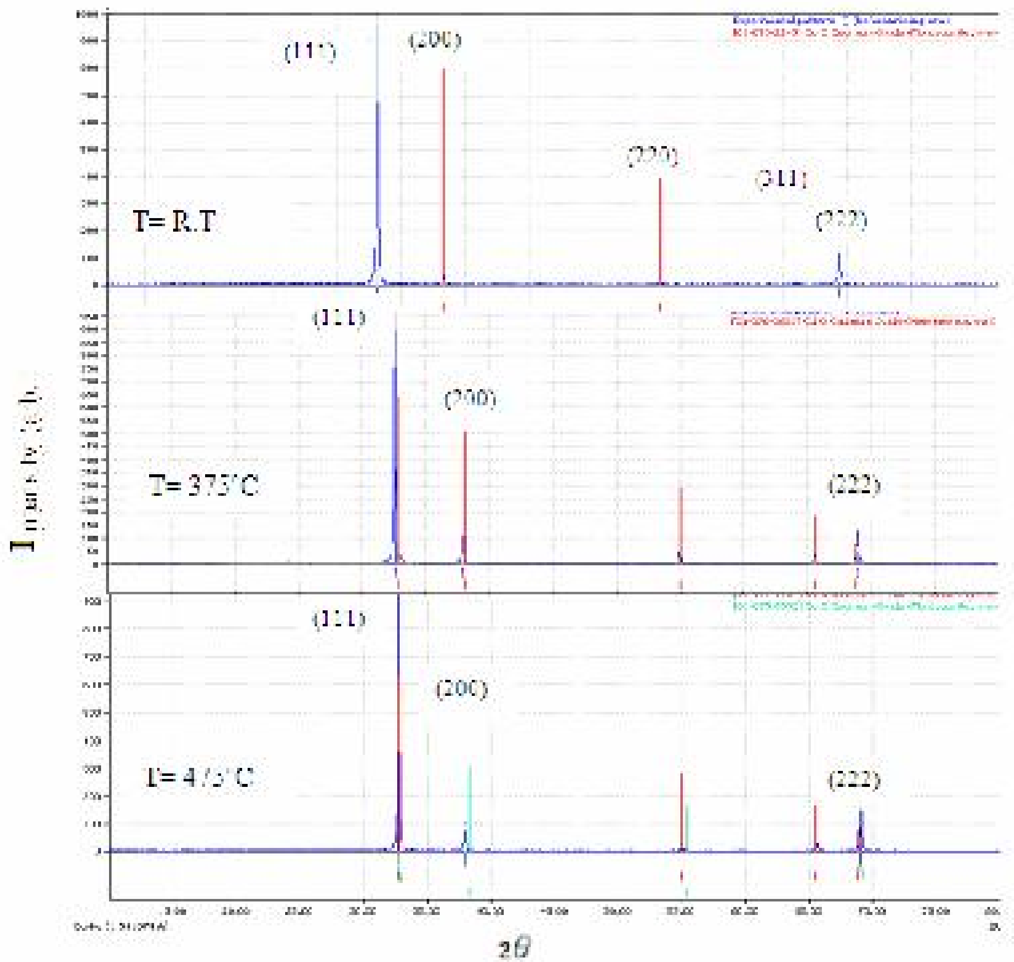

Fig.(1): X-Ray diffraction of the CdO thin films. before and after annealing temperatures

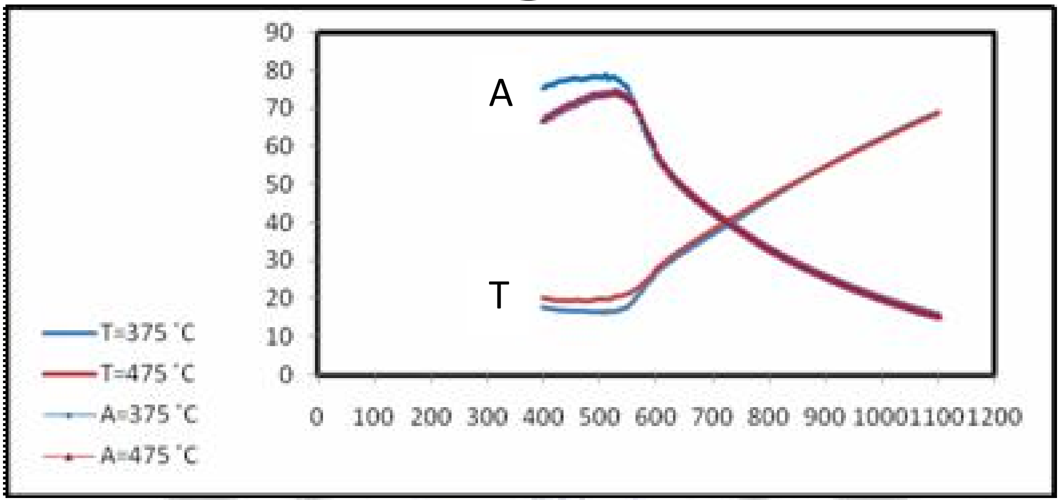

Fig.(2): Transmittance and absorbance spectra at annealing temp (375and 475) ˚C as a function of wavelength

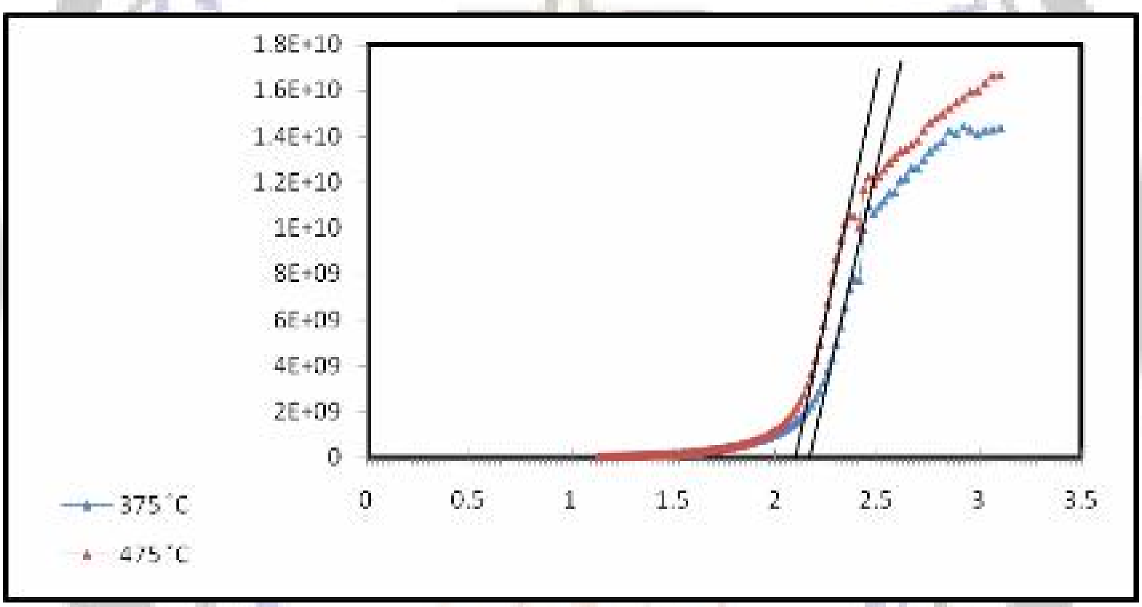

Fig.(3): The band gap is for direct transition of the CdO films at annealing temperatures: (375and 475) ˚C, and thickness: (450) nm, as a function of photon energy

تأثير درجة حرارة التلدين في الخواص التركيبية والبصرية لاغشية CdOالرقيقة المحضرة بوساطة تقنية التبخير الحراري الفراغي

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الخلاصة

حضّرت اغشية اوكسيد الكادميوم (CdO) الرقيقة بوساطة تقنية التبخير الحراري الفراغي على قواعد زجاجية بدرجة حرارة الغرفة، ودرست الخواص التركيبية والبصرية للاغشية عند التلدين بدرجة حرارة C° (375,475) بزمن ثابت مقداره ساعة واحدة ,عند السمك .nm (450) ودرس التركيب البلوري بواسطة حيود الاشعة السينية، وكانت اعلى امتصاصية عند الطول الموجي nm (530) عند درجة حرارة التلدينC° (375) التي تساوي تقريبا .(78%) وكان مقدار معدل الترسيب هو عند القيمة .nm/s (10) ووجد ان فجوة الطاقة قيمتها.eV (2.22)

الكلمات المفتاحية: اوكسيد الكادميوم، حيود الاشعة السينية، الخواص التركيبية والبصرية، الامتصاصية، فجوة الطاقة