The Effect of Thermal Annealing on the Structural and Optical Properties of CdS Thin Films Deposited by Vacuum Evaporation Method

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Abstract: Cadmium Sulphide (CdS) thin films were grown on glass substrates by the vacuum evaporation technique. The effect of thermal annealing on the structural and optical properties of the as deposited samples was analyzed. Structure of these films was characterized by X-ray diffraction. CdS films deposited have polycrystalline structure cubic (zinc blende) and hexagonal (demand). The grain size increases with increasing annealing temperature. The optical properties of CdS films have highly transmittance in visible region of spectrum and reach to more than 84%. Band gap decreases from 2.55 to 2.33 eV with the increasing annealing temperature from 473K to 623 K.

Keywords: Cadmium Sulphide, evaporation, thermal annealing, the structural and optical properties.

Introduction

The use of thin film polycrystalline semiconductors have attracted much interest in an expanding variety of applications in various electronic and optoelectronic devices. The technological interest in polycrystalline based devices are mainly caused by their low production cost[1]. Among the wide band gap II-VI semiconductors cadmium sulphide (CdS) with its direct band gap of 2.42 eV at room temperature is a promising material and is applied in wide variety of fields such as solar cells[2,3] thin film FET transistors [4], Light emitting diodes [5] and photonic devices [6]. CdS can exist in two crystalline modifications: the hexagonal (wurtzite) phase and the cubic (zincblende) phase [7].

There are various methods employed for deposition of CdS thin films such as spray pyrolysis [8], pulsed laser deposition [9], chemical bath deposition [10], electrodeposition [11], sputtering [12] and vacuum evaporation [13]. The structural and physical properties of CdS thin films prepared by vacuum evaporation technique at different deposition conditions have been reported in literature [14-17]. In this work, vacuum evaporation technique has been chosen for deposition of CdS thin films because it is a trouble-free and controllable technique. The present study is centred over the effect of thermal annealing on the structural and optical properties of thermally evaporated CdS polycrystalline thin films.

Experimental

Thin Films were prepared by the vacuum evaporation technique using Edward E306A coating unit evacuated at 10-6 mbar. Pure cadmium sulphide thin films were prepared by evaporating 99.999% pure CdS powder heated by Joule effect placed in a molybdenum boat with a controlled temperature until the material sublimates at source temperature onto glass substrates. The glass substrates were cleaned with freshly prepared acetone, detergent solution and distilled water. The source current was increased slowly (up to 90 A) and the vapor species condense onto glass substrates. The evaporation was made using the said unit at a vacuum of 5 x 10-6 mbar. The substrates were kept at 300 °K during evaporation and the substrate to source distance was kept at 17 cm. The deposition rate was maintained at 7 Å/sec. A shutter between source and substrate is used to control the thickness of the films. Film thickness was estimate to be about 1000Å. These films were then annealed in air using furnace model Yamato FM 27 at various temperatures ranging from 473 K to 623 K for a fixed time of 1 h. The X-ray diffraction(XRD) analysis was carried out using X-ray 6000(Shimadzu) diffractometer with Cuka radiation (\(\alpha\)-1.541 Å) at 40 kV and 30 mA. The
optical transmission spectra were investigated by UV-Visible Spectrophotometer (Cintra 5) GBC-Astrural).

Results and discussion

1-X-Ray Diffraction

Figure(1) shown X-ray diffraction pattern of CdS thin films deposited on glass substrate at different annealing temperature. From the diffraction pattern, it can be seen that the diffraction peak is sharp and well defined indicating that the film is polycrystalline in nature. The diffraction peak existed at 2θ = 26.5° corresponding to either the (002) hexagonal or the (111) cubic planes. From the figure, it can be seen that the intensity of diffraction peak increases as the annealing temperature of the film increase. This is an indication of the crystallinity improvement with increasing annealing temperature. These values of 2θ and its crystal planes are comparable with standard data from CdS matches well (JCPDS file no.79-0043). Similar results have been observe by literatures [18,19].

Figure (1): The X-ray diffraction patterns of CdS thin films annealed at different temperatures.

The average size of the crystallites was determined from X-ray diffraction data. We use the standard (111) C reflection at 2θ=26.5°. The Scherer formula,

\[ D = \frac{k \lambda}{\beta \cos \theta} \]

Where \( k \) is a constant taken to be 0.94, \( \lambda \) is the X-ray wavelength, \( \beta \) is the full-width at half-maximum (FWHM) of the peak, and \( \theta \) is the reflection angle[20].

The grain sizes of the CdS films increase from 20 nm to 32 nm with the increasing annealing temperature, as shown in Figure(2). Annealing thin films led to increasing in grain size because of decreases in the density of nucleation centers thus a smaller number of centers start to grow, resulting in large grains. Generally the crystallite size depends on the annealing temperature [21]. These results are consistent with other published results such as results [22,23].

Figure (2): Variation grain size with annealing temperature.
2-Optical Properties

Figure (3) shown the effect of annealing temperature on the transmission spectra in wavelength the range 400 – 800 nm. The average transmittance of the CdS films in the visible region was found to be with a transmittance of more than 84%. We have found film transmission decreases with increasing the annealing temperature.

![Graph of transmittance vs. wavelength and temperature](image)

**Fig.3. The optical transmission spectra as a function of wavelength of CdS thin films at different annealing temperature.**

Optical energy gap ($E_g$) of film was estimated from transmittance data. The photon energy ($h\nu$) and absorption coefficient ($\alpha$) for direct optical transition are related by the following equation[24].

$$ (\alpha h\nu) = B(h\nu - E_g)^{1/2} $$

Where $B$ is a constant. The curve of ($\alpha h\nu$)$^2$ vs. $h\nu$ was plotted and used to calculate the energy gap (see figure 4). It was found that the $E_g$ decreases from 2.55 eV to 2.33 eV with increasing the annealing temperature, where increasing annealing temperature causes to increasing in grain size. This decrease in the energy gap is due to the improvement in the film crystallinity. Annealing leads to sharp absorption edge because the films becomes more crystalline and the grain size increase with increase annealing temperature. These values are in good agreement with the values reported by others [25, 26]. Figure 5 show the decrease in energy gap with increasing annealing temperature.

![Graph of ($\alpha h\nu$)$^2$ vs. $h\nu$](image)

**Figure (4): A plots of ($\alpha h\nu$)$^2$ versus ($h\nu$) of CdS thin films at different annealing temperature.**
Conclusions

CdS thin films were prepared using thermal evaporation technique onto glass substrate under vacuum equal to $10^{-6}$ mbar. The X-ray diffraction studies showed that the films are polycrystalline in nature with a mixture of hexagonal and cubic phases. Grain size increase from 20 nm to 32 nm with the increasing annealing temperature. The optical transmittance measurement showed that the CdS films has flat surface, a high average transmittance over 84% in the visible region with presence of direct energy gaps decrease with increasing annealing temperature.

References

تأثير المعالمة الحرارية على الخصائص التركيبية والبصرية لأغشية Cds الرقيقية المحضرة بطريقة التبخير الفراغي

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الخلاصة
أغشية رقيقة من مادة كبريتيت الكادميوم (Cds) رستت على أرضية زجاجية بطريقة التبخير الفراغي وتم دراسة تأثير المعالمة الحرارية على الخصائص البصرية والتكيفية. الخواص التكميلية لهذه الأجسام تمكنت باستخدام تقنية جيود الأشعة السينية (XRD) حيث بنيت أن غشاء Cds يمتلك تركيبة بلورياً (كروياً) وأبعاد (ماس) معزز الحجم الحبيبي يزداد مع زيادة درجة حرارة التدفق. الخصائص البصرية دست المرسب هناك تركيبة عالية من الطيف وتصل إلى أكثر من 84% مع فجوة طاقة عريضة نقل من 2.33eV إلى 2.55eV مع زيادة درجة حرارة المعالمة الحرارية.