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Effect of Substrate Temperature on Structural and Optical Properties of Cadmium Sulfide Thin Films Prepared by Evaporation Thermal Deposition

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Abstract
In this research, we study the effect of substrate temperature (423K and 473K) on structural and optical properties for thin films of cadmium sulfide (CdS) by evaporation thermal deposition method on glass substrates and the thickness was about (390nm).XRD analysis showed that CdS thin films prepared at (423K and 473K) are single crystal and have preferred orientation along (002). The grain size was found to be increased with increasing substrate temperature, in addition, the atomic force microscopy (AFM) an increase in root mean square (RMS) with an increase in substrate temperature. The absorbance and transmittance spectra have been recorded in the range off wave length(400-800nm), and it was found that the transmittance decreases with increasing substrate temperature, while the optical band gap decreases from (2.4-2.2ev) for allowed direct transition. CdS thin films should further investigated for application towards the fabrication of solar cells.

Keywords: Cadmium sulfide, Evaporation thermal deposition method, grain size, substrate temperature, thin films, optical properties, structural properties.

الخلاصة
في هذا البحث ، قمنا بدراسة تأثير درجة حرارة الركيزة (٤٢٣ و ٤٧٣ كلفن) على الخواص التركيبية والبصرية للأغشية الرقيقة لكبريتيد الكادميوم (CdS) بواسطة طريقة الترسيب بالتبخير الحراري على ركائز الزجاج حيث كان سمك الغشاء حوالي ٣٩٠ نانومتر . أظهر تحليل حيود الاشعة السينية XRD أن أغشية كبريتيد الكادميوم CdS الرقيقة التي تم إعدادها في درجة حرارة (٤٢٣ و ٤٧٣ كلفن) هي ذات بلورة منفردة ولها اتجاه مفضل على طول (٠٠٢). وجد بان الحجم الحبيبي يزداد مع زيادة درجة حرارة الركيزة ، بالإضافة إلى ذلك ، فإن مجهر القوة الذرية (AFM) اضهر زيادة في معدل مربع الجذر التربيعي (RMS) عند زيادة درجة حرارة الركيزة. تم تسجيل اطياف الامتصاصية والنفاذية في مدى نطاق الموجة (٤٠٠-٨٠٠) نانومتر، وتبين أن النفاذية تقل مع زيادة درجة حرارة الركيزة ، في حين تنخفض فجوة الطاقة

Introduction
Cadmium sulfide is member of II-VI group of semiconductors. CdS that has a yellow – orange color, and two – crystal structures, cubic and hexagonal closed Packed (wurtzite) phases. The nearest neighbor bond lengths Cd–S is closely equal in the both cubic and hexagonal crystal structure. This has a direct gap of about (2.4 eV). It exists near the photon energy of maximum solar radiation spectrum; it causes absorption in the short wavelength side, and has a high absorption coefficient within the solar radiation to generate carriers across the band gap with wavelength less than (520 nm). CdS is used as low-cost photovoltaic devices and usually used as a very suitable window layers that are prepared as thin as possible to avoid optical transition losses. Several methods have been employed to deposit thin films for different applications like chemical path deposition [1], electro deposition [2], spray paralysis [3], vacuum evaporation [4]. Among these, vacuum evaporation technique is a well-established technique for the preparation of uniform films with good crystallinity. The physical properties of the films prepared by vacuum

evaporation technique depend on many factors such as film thickness, substrate temperature and deposition rate [5]. CdS thin films are deposited by vacuum evaporation at different substrate temperatures and the films are characterized by several techniques such as X-ray diffraction, Scanning Electron Microscopy and optical transmittance. In addition, the effect of substrate temperature on the structural and optical properties is discussed. The aim of this work is to grow cheaper and more efficient CdS. The decorative applications of thin films will also be considered in addition to their applications in agriculture, electronics and optoelectronic devices.

Materials and Methodology

In this research, the evaporation thermal deposition system type (Edward 305 Unit) has been used to synthesis CdS thin films on glass substrate with different temperature 423K and 473K. Glass substrates made from slide microscopes manufactured in Germany in "Objekttrager Factory" which dimensions cutes with (1.25x1) cm^2. They washed by soap and tap water very well to remove any oil or dust on the substrate surface and immersed in a pure alcohol solution which reacts with contamination such as grease and some oxides; this process is achieved accurately by washing the substrates in ultrasonic for 15 min. Eventually the slides were dried and exposed to blowing air wiped with soft or Optical paper, and then the slides will be ready to be used. The material of CdS placed inside chamber evacuated to 10^{-5} mbar in a resistive heater in a form of a boat have high melting point made of tungsten connected to electric source. The distance between the substrates and boat are (10.95 cm). Thickness is one of the most important parameters in thin films. Here we use weight method to measure thickness as the following: The film thickness (t) can be measured by evaporating certain weight (m) of material, if the distance between the evaporation boat and the substrate was (r) and the density of material in its bulk was (ρ). Thus, the film thickness is given by the following equation [6]:

$$t = \frac{m}{2\pi\rho r^2} \tag{1}$$

Structural measurements

As described in this work, X-ray diffraction has been used to study the structural and morphological of thermally evaporated CdS thin films. It is found from Figures (1) and (2) determined using x-ray diffraction at substrate temperature 423Kand 473K respectively.

Both samples deposited were single crystalline consisting of hexagonal phase, comprising a strong reflection along (002) preferred plane at 2θ=26.930 and that at 473K while at was 2θ=26.892. It was found that the position of (002) diffraction peak change among the two temperature values by about (0.038°). This may attributed to the change in internal stress of the films at various temperatures during film growth. The degree of preferred orientation decreased with the substrate temperature thus, raising the temperature did not lead to the formation of other planes.

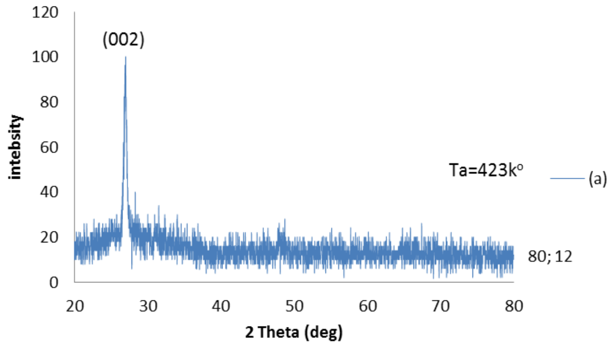

Figure 1: X-ray diffraction spectrum for CdS thin films deposited at substrate temperature 423K.

In fact, the film prepared at higher temperature, has a better crystalline quality as indicated from X-ray spectra see Figure 2.

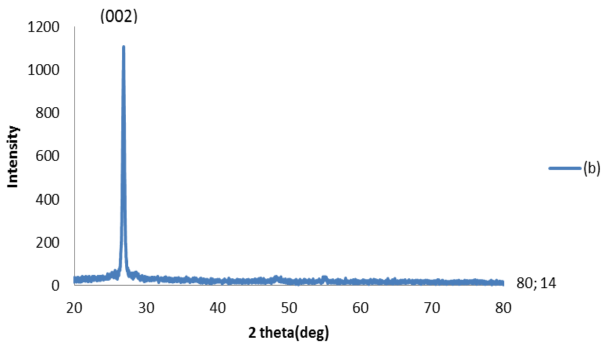

Figure 2: X-ray diffraction spectrum for CdS thin films deposited at substrate temperature 473K.

The X-ray parameters can be summarized in Table 1:

Table 1: X-ray parameters of CdS thin films at different substrate temperatures.

Temperature (K)	423K	473K
2θ	26.9302	26.8924
d(Å)	3.30810	3.31266
FWHM	0.43500	0.31820
I(count)	45	658
I/I_1(ASTM)	100	100

The effect of substrate temperature on the grain size can be calculated from the obtained phase can be investigating simply from the (002) diffraction line using Scherer's formula equation:

$$D_g = \frac{k\lambda}{\beta cos\phi} \quad (2)$$

Where k is constant taken as (0.9), λ: is the wavelength of incident X-ray radiation = (1.5404Å for CuKα), β is the full width at half maximum for (26.930).
The grain size increases from 20nm to 40nm with increases substrate temperature. Increasing the substrate temperature led to the increasing in grain size because of the decrease in the density nucleation centers the smaller number of centers starts to grow up, resulting in large grains. Generally the crystalline size depends on the temperature.
Atomic Force Microscopy (AFM) is a characterization, with high resolution, that is applied for the investigation of the surface topography in the nanometers scale. The main advantage of AFM is its sub-nanometer resolution and the possibility to give a direct real space image of the surface because there is no current flow , the AFM can be used on electrically conductive or non-conductive surface and in the vacuum or fluid environment. AFM resulting information yield imaging with statistical information about surface roughness depending on the root mean square (RMS).These fine imaging in 2-D and3-D properties. Figure 3 and 4 show the AFM results of CdS thin films at deposition temperature 423K and 473K.
AFM results shown in Figures (3and 4) can be tabulated in Table 2 obtained from CdS thin films thermally deposited on glass substrate and different substrate temperature, showing the average grain size and roughness values.

Table 2: AFM parameters of CdS thin films prepared at different temperatures.

Substrate temperature (K)	Average grain Size (nm)	RMS (nm)
423	11.3	0.913
473	56	2.85

It can be noticed that the grain size and RMS for thermally evaporated CdS thin films are increased with increasing substrate temperature, which is in agreement with [7]. These result indicated that these films will be suitable for solar cell application. Hence, as temperature increased grain size and crystalline getting better due to the rearrangements of grain size in the crystal.
The SEM image of CdS thin film Figure 5 and 6 show that the films are conquered on glass substrate from a kind of cracks on the surface of the films. Al thought there is difference in grain size revealed 20nm at 423K to 40nm at 473K respectively. The grain size calculated by SEM is slightly greater than the values of grain is close agreement with [8].

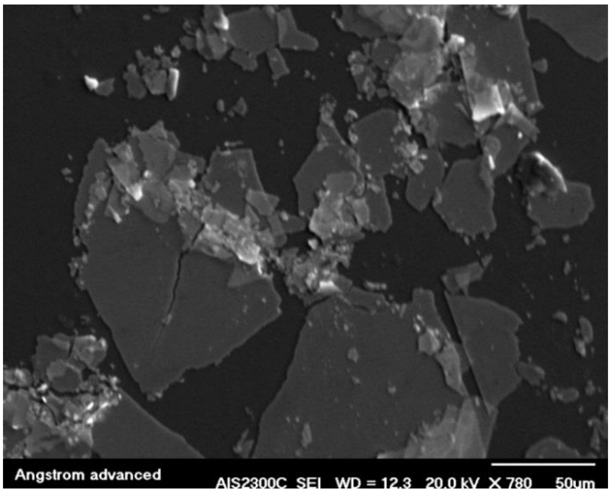

Figure 5: SEM image of CdS thin films prepared at 423K.

Optical measurements

Nanostructure thin Films obtained by using the UV-Vis photo spectrophotometer.

Figure 7 shows the variation of optical transmission as a Function of wave length in the range of (400-800)nm in the visible region which is very suitable for solar cell. The value for the films prepared at different deposition temperature at T_a=423K and T_b=473K, respectively. It can be noticed that the film at low temperature have high transmission and that film prepared at higher temperature have a lower transmittance[9]. It can be observed that in general an increase in substrate temperature due to the less defect and scattering and improvement crystalline microstructure of the films as the temperature increases, the surface roughness and density of localized state increases which reduces the transmission value.

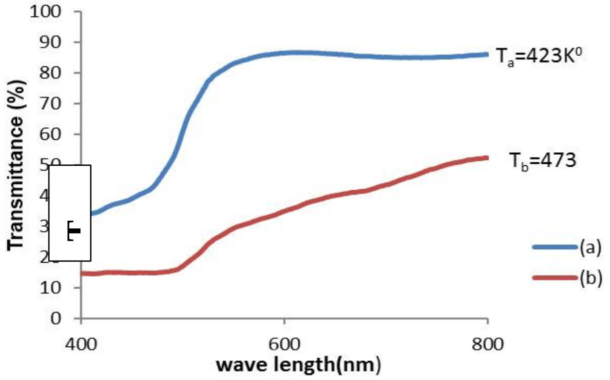

Figure 7: Transmission spectra of CdS thin film at different deposition temperature T_a at 423K and T_b at 473K, respectively.

The visible spectrum shows a minimums absorption, that is mean that the films is suitable to be antireflection coating. At high wave length, the incident photon does not have enough energy to interact with atoms, thus the photon will be transmitted when wave length decrease (photon energy increases). The interaction between incident light and material will be occurred and then the absorption will increase. Figure 8 absorption spectra at different deposition temperature T_a at 423K and T_b at 473K, the fast increase in absorption below 400nm, may be attributed to absorption of light caused by excitation of electrons from the valence band to the conduction band of CdS. While the high region observed for this thin film is due to the fact that they have a rather high energy band gap~2.42eV. This will reduce absorption in the visible range and make it as transparent material.

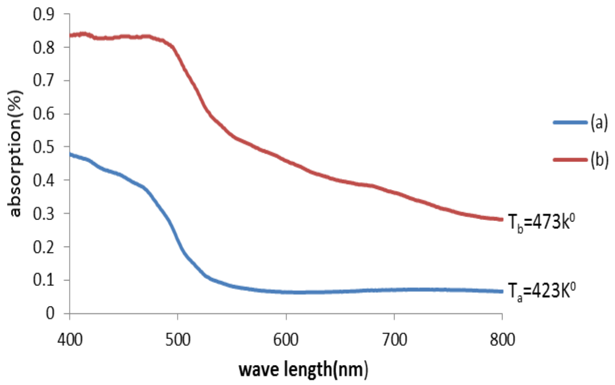

Figure 8: absorption spectra at different deposition temperature T_a at 423K and T_b at 473K, respectively.

Figure 9 represents the evaluation of E_g from $(\alpha hv)^2$ versus photon energy for different deposition temperature T_a at 423K and T_b at 473K, respectively.

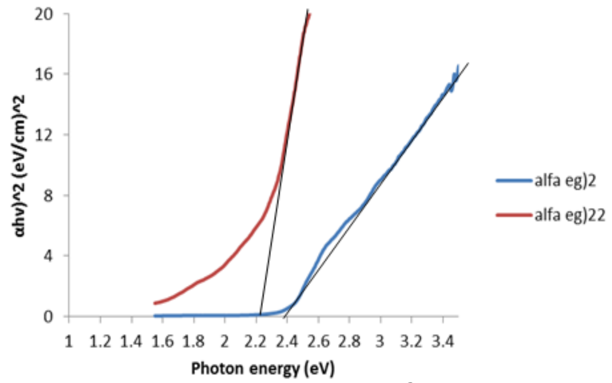

Figure 9: The relation between $(\alpha h\upsilon)^2$ with $(h\upsilon)$ for CdS at different deposition temperature T_a at 423K and T_b at 473K, respectively.

The energy gap values depend in general on the films crystal structure, the arrangement and distribution of atomic in the crystal lattice, also by crystal regularity. It was found in literature that CdS thin films has a direct band gap which values changed slightly according to the parameters and conditions.

It can be seen from Figure 9 that the allowed directed energy band gap decreased from E_g=2.4eV at 423K temperature to E_g=2.2eV at 473K. This decreased with temperature can be attributed to the improvement of crystallinity and enlargement of grain size. This can be explained by better crystallization and greater grain size take place in the films, which leads to the decreases in the decreases in the defects density and crystal density and the crystal – boundary.

Conclusions

The influence of substrate temperature increase achieved many results: The film has a good optical well-suited for solar cell application. Also, Proved the Structure measurements to Prepared films at temperatures(423K and 473K) by thermal vacuum deposition method they are structure single crystal at (002) type of Hexagonal. Increase in temperature lead to an improvement in the crystalline case any increase grain size. Grain size values recorded on the structures within the beloved compositions nanoparticles show and this is what trailed the results of X-rays. The results of optical measurements proved that transmission of films decreases with increasing temperature.

References

[1] H. Moualkia, S. Hariech, and M. Aida, "Structural and optical properties of CdS thin films grown by chemical bath deposition," *Thin Solid Films,* vol. 518, pp. 1259-1262, 2009.
[2] S. Mondal, A. Dhar, and S. Ray, "Optical properties of CdS nanowires prepared by dc electrochemical deposition in porous alumina template," *Materials Science in Semiconductor Processing,* vol. 10, pp. 185-193, 2007.
[3] K. Ravichandran and P. Philominathan, "Investigations on microstructural and optical properties of CdS films fabricated by a low-cost, simplified spray technique using perfume atomizer for solar cell applications," *Solar Energy,* vol. 82, pp. 1062-1066, 2008.
[4] K. Senthil, D. Mangalaraj, S. K. Narayandass, and S. Adachi, "Optical constants of vacuum-evaporated cadmium sulphide thin films measured by spectroscopic ellipsometry," *Materials Science and Engineering: B,* vol. 78, pp. 53-58, 2000.
[5] M. Tomakin, M. Altunbaş, E. Bacaksiz, and Ş. Çelik, "Current transport mechanism in CdS thin films prepared by vacuum evaporation method at substrate temperatures below room temperature," *Thin Solid Films*, vol. 520, pp. 2532-2536, 2012.
[6] K. L. Chopra and I. Kaur, "Magnetic Thin Film Devices," in *Thin Film Device Applications*, ed: Springer, 1983, pp. 171-197.
[7] U. Pal, R. Silva-Gonzalez, G. Martinez-Montes, M. Gracia-Jimenez, M. Vidal, and S. Torres, "Optical characterization of vacuum evaporated cadmium sulfide films," *Thin solid films,* vol. 305, pp. 345-350, 1997.
[8] M. Kale, Y. Toda, M. Bhole, and D. Bhavsar, "Structural, optical and thermo electrical properties of nanostructured vacuum evaporated CdS thin films," *Electronic Materials Letters,* vol. 10, pp. 21-25, 2014.
[9] V. Gevorgyan, L. Hakhoyan, N. Mangasaryan, and P. Gladyshev, "Substrate Temperature and Annealing Effects on the Structural and Optical Properties of Nano-CdS Films Deposited by Vacuum Flash Evaporation Technique," *Chalcogenide Letters,* vol. 13, pp. 331-338, 2016.