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Structure and Optical Properties of the $CdS/Cd_{2x}(CuIn)_{1-x}S_2$Heterojunction Prepared by Chemical Spray Pyrolysis

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Abstract: The structural and optical properties of the CdS, $Cd_{2x}(CuIn)_{1-x}S_2$ (CCIS) thin films, at x=0.2,heterojunction were studied in the present paper. The heterojunction films deposited successfully on glass slides using by the spray pyrolysis technique at 623K. The thin films CdS, CCIS and the heterojunction ITO/CdS/CCIS were characterized by using x-ray diffraction. This is to find the polycrystalline series of the CdS, and CCIS solid solution with many phases as a mixture of chalcopyrite and zinc blend. The CdS, and CCIS thin films have a grain size 35 nm, and 16 nm respectively. The surface morphology was characterized by using atomic force microscopy (AFM) technique. The optical properties of the prepared thin films were investigated by using a UV-VIS spectrophotometer in the wavelength of 300 nm to 1100 nm. The films, ITO, CdS, and CCIS show direct transition with optical energy gap (Eg) values 3.52, 2.42, and 1.7eV respectively. The optical transmission (T),absorption (A) andrefractive index (n) were also discussed
.

Keywords: *The ITO/CdS/$Cd_{2x}(CuIn)_{1-x}S_2$Structure, Optical, heterojunction and thin films..*

I. INTRODUCTION

The chalcopyrite compound copper indium disulfide, $CuInS_2$, is one of the most promising candidates to substitute $CuInSe_2$ as absorber material for photovoltaic applications[1]. Solar cell compounds such as $Cu(In_{1-x}Ga_x)Se2$, CuInSe2(CISe), and CuInS2 (CIS) have received much attention from research groups around the world because of their potential properties, such as high efficiency, reliability, and stability[2] . Most of the reported studies are on the development of heterojunction between p-type CuInS2 and n-CdS[3-5].Thin CdS films are deposited as intermediate layers to improve the interface properties and a chemical buffer layer to protect the CuInS2 or CdTe during the subsequent processing .[6] Therefore, phase relations involving CuInS2 and CdS have to be investigated to assess possible element inter-diffusion at the p-n hetrojunction and to provide additional information on solid solution and possible intermediate phases [7].Thus, by taking the similarity of their crystalline structures into account, CdS doped with CuInS2 to form $(CuIn)_xCd_{2(1-x)}S_2$complexs which could be identified for improving the photocatalytic activity and stability of CdS [8]. Many techniques including electrodeposition [9], spray pyrolysis [2], vacuum evaporation [10], and chemical bath deposition CBD [11], have been used to produce the device layers [6]. Theaim of the projectisto prepare ITO/CdS/$Cd_{2x}(CuIn)_{1-x}S_2$heterojunction through spray pyrolysis and to study its structure, and optical properties.

II. EXPERMENTAL

TheITO/CdS/$Cd_{2x}(CuIn)_{1-x}S_2$heterojunction, with x=0.2, was prepared via chemical spray pyrolysis. The indium tin oxide (ITO), CdS, and $Cd_{2x}(CuIn)_{1-x}S_2$ thin films were prepared by mixing 0.1M and spraying an aqueous solution of ($InCl_3$, $Sncl_2$) to obtained ITO, deposited on micro glass slides which were first cleaned with detergent water and then dipped in acetone.The cadmium sulfide CdS ($CdCl_2$, thiourea $[CS(NH_2)_2]$), at ratio 1:1 deposited on ITO, and $Cd_{2X}(CuIn)_{1-x}S_2$ ($CdCl_2$, $CuCl_2$, $InCl_3$, thiourea $[CS(NH_2)_2]$) at ratio 0.4:0.8:0.8:2, deposited on CdS. The distance between the nozzle and the substrate at 45 cm. The automated spray solution is transferred to the het substrate could be kept at the normalized deposition temperature of 623K by using filtered air as carrier gas at a flow rate normalized to approximately 3 ml/min. To prevent the substrate from excessively cooling, we sprayed the prepared solution on the substrate for 10s with 15s intervals. Using the optical method, we measured the thicknesses of the films of heterojunction, ITO at 300 nm, CdS at 350 nm, and CCIS at 910 nm. The nature of the growth and structure characteristics of the prepared thin films and heterojunction were determined via X-ray diffraction(XRD) by using a Philips PW1840 diffractometer with Cu-Kα target. The morphology of the films was determined via atomic force microscopy (AFM) (AA 3000; Angstrom Advanced Inc.). The UV-VIS spectrophotometer (Tenway 6800 UV-VIS) was used to measure the absorptance and transmittance in the wavelength range of 300 nm to 1100 nm, and from these measurements, the optical parameters were calculated.

III. RESULTS AND DISCUSSION

In order to study the characterization of each layer of the heterojunction solar cell, these layers were deposited on glass slides, so the structural and optical were studied and correlated with preparation parameters to optimize the best conditions fitting the solar cell performance.

A. XRD analysis and surface morphology

The structure of the prepared thin films and the heterojunction were examined via XRD. Fig. 1 shows that the polycrystalline film $Cd_{2x}(CuIn)_{1-x}S_2$ at x=0.2 has $CuInS_2$, CdS, In_2S_3, and CCIS peak, indicating that the $Cd_{2x}(CuIn)_{1-x}S_2$ system forms a solid solution. This is similar to the observed by Ren et al.[8],Marushko et al.[12], and Hamid et al.[13]. The analysis of the XRD patterns shows that the $CuInS_2$ structure is a tetragonal chalcopyrite phase and a hexagonal or cubic phase for CdS as shown in Fig. 1, this is similar to the observed by A.AYadav et al.[14]. The average grain size of the CCIS, and CdSis calculated from the full width at half maximum (FWHM) of the (101) line of the film, byusing the scherrer formula [15] were 16, and 35 nm, respectively.These results agree with those of Ravichandran et al.[16], and

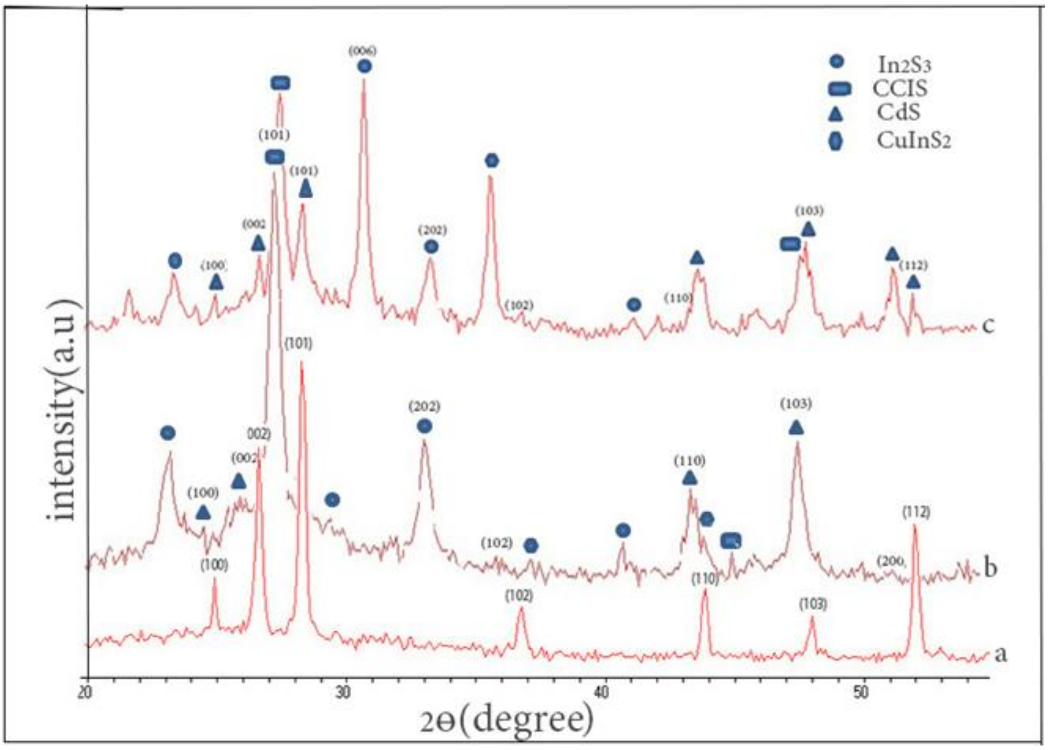

Fig. 1. X-ray diffraction patterns (a) CdS, (b) CCIS, and (c) ITO/CdS/CCIS

Ashour[17]. Fig. 1also shows that the heterojunction structure has $CuInS_2$, CdS, In_2S_3, and CCIS peaks.The average grain size of CCIS is calculated from (FWHM) of the (101), and (002) by using the scherrer formula [15] 27, and 11, respectively. Typical CCIS film with x=0.2 and CdS film were morphologically characterized by using the AFM, as shown in Fig. 2,photographs of the films. The root mean square values of the surface roughness of CdS, and CCIS films are5.4, and 14.1 nm/2µm x 2µm, respectively.

B. Optical Properties

The optical absorption and transmission spectra of CCIS, CdS, and ITO films were recorded in the 300 nm to 1100 nm range. The transmission (T) spectra are important parameter for optical materials and applications. The T value which depends on wavelength (λ) is shown in Fig.3. The peak values of T of the films, ITO, CdS, ITO/CdS are equal 75%, 70%, 58% respectively. The absorption coefficient (α) was calculated using the following relation:

$$\alpha = 2.3\frac{A}{t} \qquad (1)$$

where *A* is absorption and *t* is the film thickness.. Fig . 4 shows that the plot of α is the versus to the wavelength λ of the films that have high values ($\alpha > 10^4\ cm^{-1}$) at visible range and then become nearly constant at NIR range.

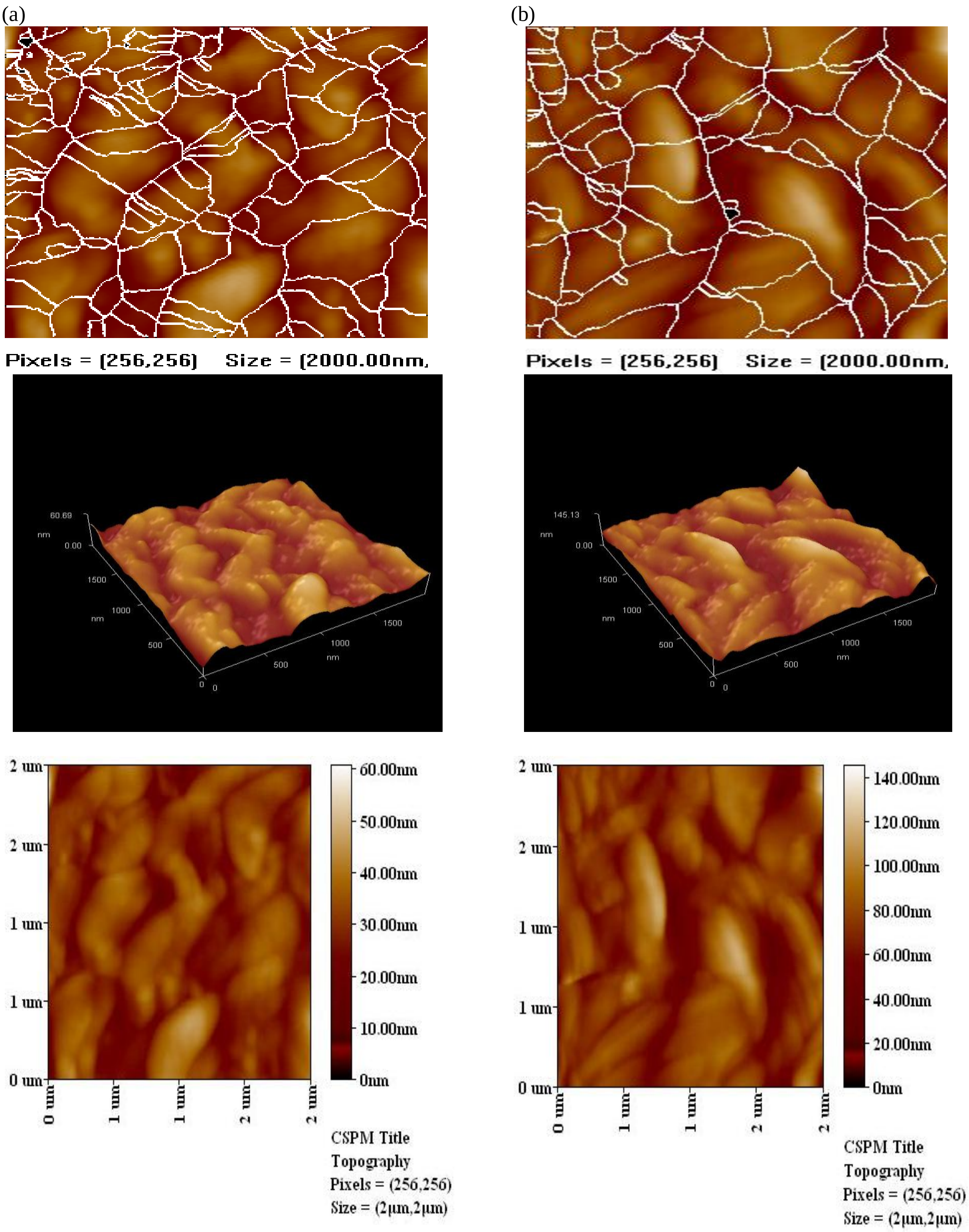

Fig. 2. AFM photographs of (a) CdS, and (b) CCIS.

The energy band gap of the films can be estimated from the tangent line in the plot of $(\alpha hv)^2$ with hυ (fig.5). The band gaps of $CuInS_2$,ITO, and CdS are 1.4, 3.6eV, and 2.4eV respectively [8,18,19]. The energy gap of the films, CCIS, ITO, and CdSare 1.7, 3.52, and 2.42eVrespectively.

3. The transmission of (a) CdS, (b) ITO, and (c) ITO/CdS.

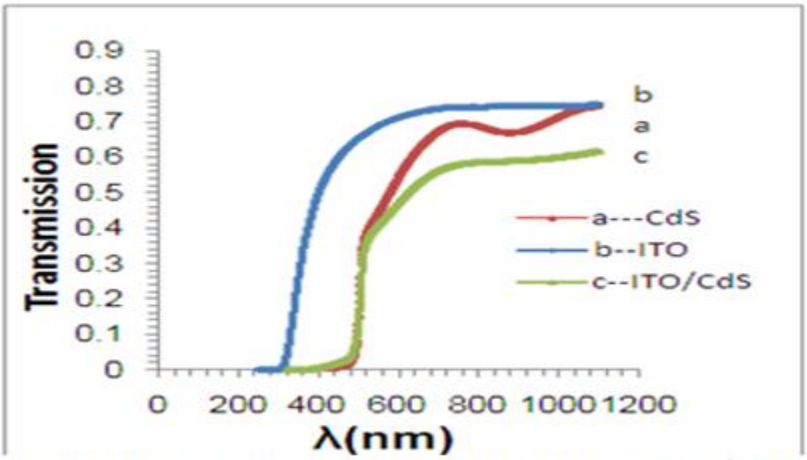

Fig. 3. The transmission of (a) CdS, (b) ITO, and (c) ITO/CdS.

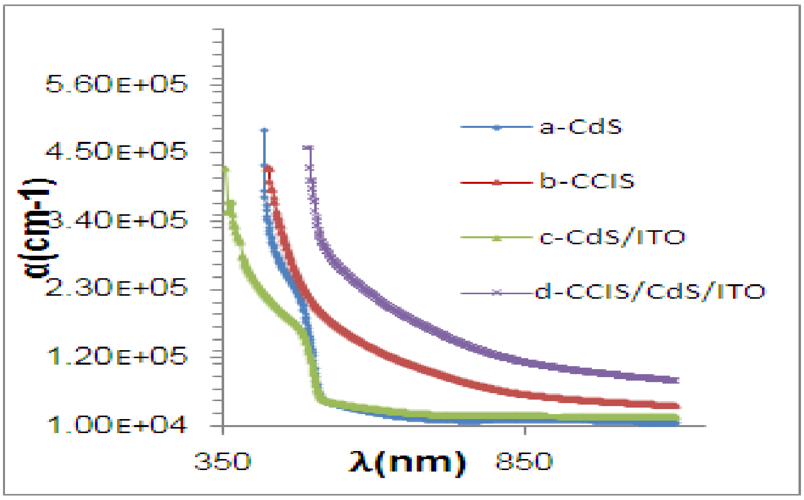

Fig. 4. The absorption coefficient (α) vs wavelength (λ) for (a) CdS, (b) CCIS, (c) ITO/CdS, and (d) ITO/CdS/CCIS.

The refractive index (n) value which depends on hυ, is shown in Fig. 6.The peak values of n of the films, CCIS, CdS, and ITO/CdS are equal 1.8, 2.6,and 2.5 respectively.

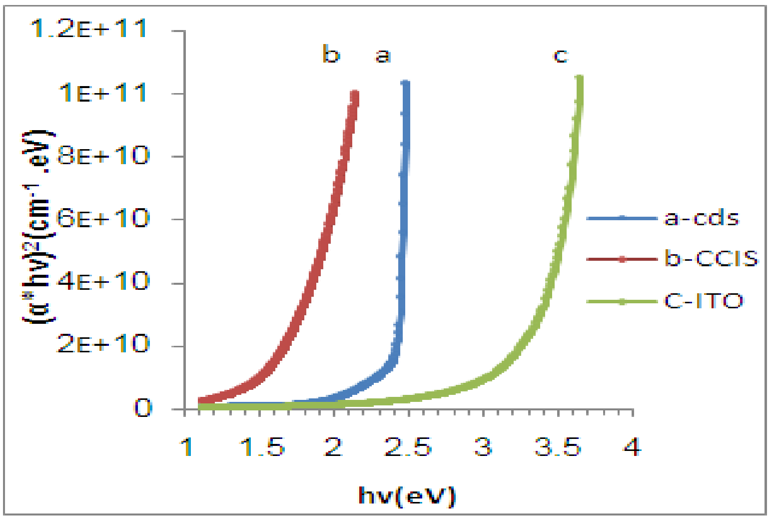

Fig. 5. The energy gap of the films, (a) CdS, (b) CCIS, and (c) ITO.

The extinction coefficient (k) value which depend on hυ, is shown in Fig.6. The peak values of k of the films CdS, CCIS, and ITO/CdS were 1.2, 1.3, and 0.9, respectively shows in Fig. 7.

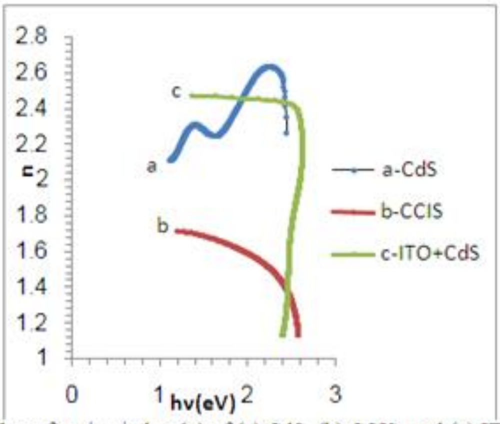

Fig. 6.The refractive index (n) of (a) CdS, (b) CCIS, and (c) IT(

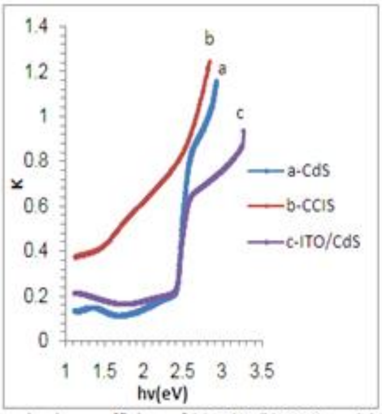

Fig. 7. The extinction coefficient of (a) CdS, (b) CCIS, and (c) ITO CdS.

IV. CONCLUSIONS

The device ITO/CdS/CCIS was synthesized by using a simple chemical spray pyrolysis technique. The XRD shows that the film CdS have hexagonal and cubic structure, and the CCIS film has $CuInS_2$ crystals in the chalcopyrite structure and CdS crystal and the hexagonal structure. The optical studies show that the films, ITO, CdS, and CCIS have direct optical energy gap 3.52, 4.42, and 1.6 eV. The surface morphology studies by AFM.

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