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Structural Properties of CdS Thin-films Deposited by RF Magnetron Sputtering

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***Abstract*—Cadmium Sulfide (CdS) thin-films were deposited by RF magnetron sputtering at different RF power ambient and their structural properties were studied to observe the effect of different sputtering conditions on the structural properties of CdS films. CdS is widely used buffer layer for chalcopyrite based photovoltaic cells and requires good crystalline property and less dislocation density as well as strain in conjunction with a thinner layer ensures good crystalline quality. The as deposited films were characterized by X-ray diffraction and the structural properties (crystal type, lattice alignment, lattice constant, crystalline size, microstrain, dislocation density, etc.) were analyzed. Analysis on structural properties shows that crystallite size increases and crystalline quality enhanced with higher RF power, while the dislocation density and developed strain declined for the same conditions. This investigation concluded that higher RF power sputtered CdS thin-films for lower time deposition can be more suitable for thin-film photovoltaic cell applications.**

Keywords— RF Sputtering, thin-films, CdS buffer layer, X-ray diffraction, crystal structure, photovoltaic cell applications.

I. Introduction

Direct bandgap group II-VI compound semiconductor material Cadmium Sulfide (CdS) is one of the most comprehensively utilized materials in optoelectronic devices as well as photovoltaic (PV) cells. N type CdS material has some basic structural and optoelectronic properties like wide bandgap, high transparency and the possibility of heavy doping ($\sim 10^{19}$ cm^{-3}) make it as a good kind of n type heteropartner for thin-film PV cells. As of late, broad research on the synthesis and characterization of CdS thin-films has been done because of its promising applications in thin-film PV cells [1][2].

Several methods of synthesis techniques are accessible to deposit CdS thin-films such as sputtering [2][3] (Radio Frequency, DC, Pulsed DC), chemical bath deposition [4], thermal evaporation [5], closed space sublimation [6], Spray pyrolysis [7], Chemical vapor deposition [8] and so on. Among those techniques, radio frequency (RF) sputtering is one of the most dependable systems utilized in the synthesis of polycrystalline CdS thin-films and permitting a decent control of film consistency, thickness and crystalinity over enormous territory substrates [9][10]. The process ambient conditions, base pressure, operating pressure, process temperature, RF power and target to substrate distance are the important parameters for sputtered deposition of thin-films which influence the electrical, optical, structural and so many physical properties of the deposited films.

This work demonstrated structural and crystalline properties of CdS thin-films fabricated by RF magnetron sputtering. By varying the RF power, while all the process parameters were kept constant, the effects of RF power on the structural properties of as deposited CdS thin-films have been studied.

II. Experimental Details

Thin-film CdS were sputtered on bare soda lime glass substrate (SLG) from high purity CdS sputtering target of 2 inch diameter and 0.25 inch thickness with 99.99% purity (from Kurt J. Lesker Company). Nano master NSC-3500 2 gun RF sputtering machine was used for sputtered deposition of CdS thin-films.

Experiments were performed at 100˚C fixed substrate temperature. High purity Argon gas was used as process gas. Base pressure was maintained at 5×10^{-5} Torr and the working pressure during deposition was maintained at 2.3 mT by process gas flow rate of 10 SCCM. The distance between target to substrate was kept fixed 80 mm for all experiments. The sputtering power was varied for deposition of CdS thin-films where all the process parameters were kept constant. The target was covered by shutter and pre-sputtered at 50 W RF power prior to deposition to get rid from the unwanted oxide content and other contaminations on the target surface.

Prior to deposition, the SLG substrates were cleaned by a sequential MAMD (MAMD stands for Methanol Acetone Methanol Deionized water) process. Firstly glass substrates were mechanically scribed into diluted liquid soap solution and then rinsed with double deionized (DI) water. Afterwards the substrates were soaked into 5% diluted HCL and rinsed with DI water. Then the substrates were processed to clean sequentially in ultrasound bath for 10 minutes with methanol, acetone, methanol and DI water. All the ultrasound cleaning processes except DI water cleaning were performed at room temperature where the ultrasound cleaning with DI water was

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performed at 60˚C. After processing of all the cleaning steps, the substrates were dried by pure industrial nitrogen gas and further baked in air at 100˚C.

Four set of samples were deposited by varying the RF power 30 watt (S1), 40 watt (S2), 50 watt (S3) and 60 watt (S4) while all the process parameters were kept constant as described before. Deposition time was kept fixed 1 hour for all experiment sets. The samples were naturally cooled to room temperature under vacuum after deposition. The deposited samples at different RF power are shown in Fig.1.

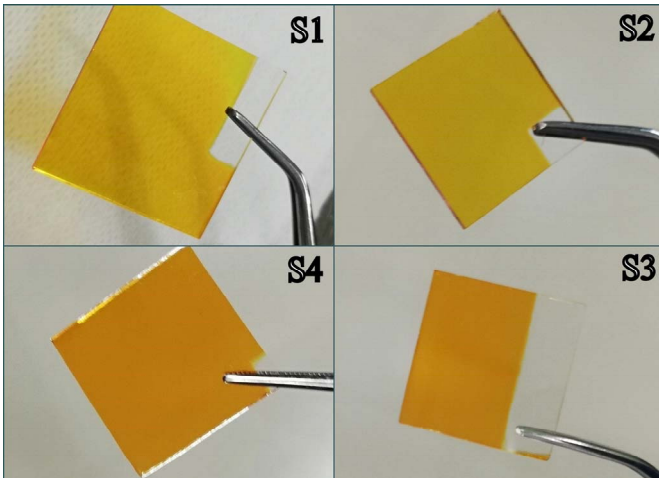

Fig. 1. RF Sputtered CdS thin-films (S1,S2,S3 and S4) fabricated at various RF power

Quartz crystal monitor (QCM) gives the approximate measurement of deposited film thickness and the QCM readings for the samples are shown in TABLE I.

The TABLE I data show that the deposition rate increases linearly with RF power at a slope 0.48617 nm/min/watt. The linear fit of RF power versus deposition rate is shown in Fig.2.

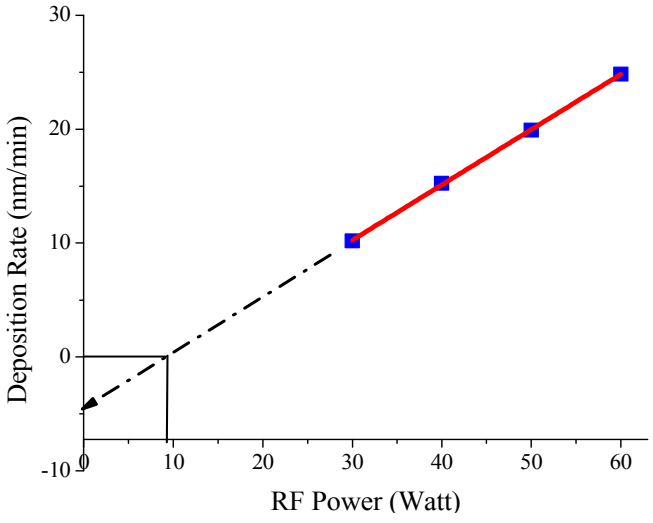

Fig. 2. Linear fit of deposition rate versus RF power for this work

So as to explore the structural properties of CdS thin-films fabricated at various power, fabricated films were further analyzed through X-ray diffraction (XRD) spectrum using Empyrean, PANalytical-Netherlands diffractometer with CuK_α radiation, λ=0.15405 nm and Crystallographic properties (grain size, micro strain, crystal planes, dislocation density and lattice type) were calculated and analyzed.

TABLE I. QUARTZ CRYSTAL MONITOR READING FOR THE FABRICATED CdS THIN FILMS AT DIFFERENT RF POWER

Sample Name	RF Power (Watt)	QCM Reading (nm)	Deposition Rate (nm/min)
S1	30	611	10.18
S2	40	915	15.25
S3	50	1195	19.91
S4	60	1490	24.83

III. RESULTS AND DISCUSSIONS

Structural parameters as well as lattice parameters of RF sputtered CdS are calculated from the XRD spectrum and the effects of variation of RF power on structural parameters are observed while all the deposition parameters are kept constant as described above. Lattice constant, a for hexagonal structure has been computed using Brag's law and in some case Vegard's linear approximation as in (1)-(4) [11][12]. The calculated parameters are assigned in Table I.

$$a_{cubic} = d_{hkl}\sqrt{h^2 + k^2 + l^2} \quad (1)$$

$$a_{hex} = a_{cubic}\sqrt{0.5} \quad (2)$$

$$C_{hex} = \alpha_{cubic}\sqrt{\left(\frac{4}{3}\right)} \quad (3)$$

$$d_{hkl} = \frac{\lambda}{2 \times \sin\theta} \quad (4)$$

Where, λ is CuKα X-ray radiation wavelength (0.15406 nm), d is inter planar spacing in the lattice and θ is the angle between incident X-ray and scattering plane. Average grain size (D), micro strain(C) and dislocation density (δ) in the CdS crystal can be estimated from XRD pattern by applying Debye-Scherrer formula as in (5)-(7) [12] as assigned in Table II.

$$\text{Crystallite (Grain) size, } D = \frac{0.9\lambda}{(\text{Full Width Half Maxima}) \times \cos\theta} \quad (5)$$

$$\text{Micro strain, } C = \frac{(\text{Full Width Half Maxima})}{4\tan\theta} \quad (6)$$

$$\text{Dislocation density, } \delta = \frac{15C}{aD} \quad (7)$$

TABLE II. SUMMARY OF CRYSTALLOGRAPHIC PARAMETERS OF RF SPUTTERED CdS THIN-FILMS

Sample Name	Avg. Crystallite Size (nm)	Micro Strain, $C(\times10^{-3})$	Lattice Constant, a (Å)	Dislocation Density δ ($\times10^{12}$ cm^{-2})
S1	27.17	4.12	5.846	0.389
S2	32.32	3.72	5.836	0.296
S3	32.57	3.48	5.838	0.275
S4	33.63	3.48	5.835	0.266

XRD spectrum of as deposited CdS thin-films fabricated at different RF power are shown in Fig.3. Multiple diffraction peaks demonstrated that the nature of the as deposited CdS thin films is polycrystalline. A very sharp dominant peak has observed at 2θ = 26.4˚ and another peak has observed at 2θ = 54.45˚. From the JCPDS card number 77-2306, the characteristics peaks indicate cubic structure and correspond to plane (111) and (222).

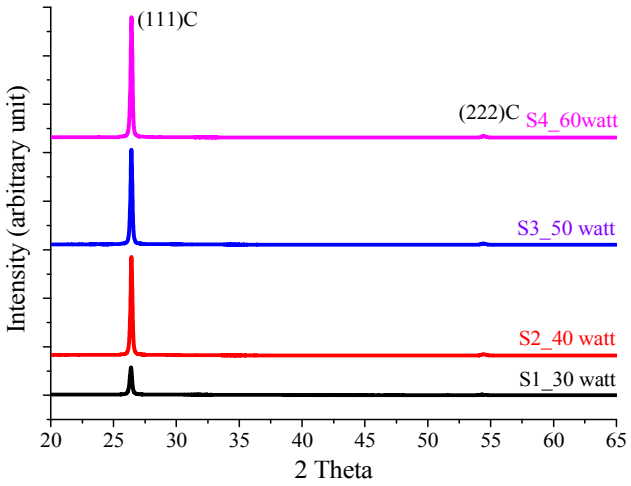

Fig. 3. XRD spectrum of RF sputtered CdS thin-films

The lattice constant data (a ~ 5.83 **Å,** which is matched with lattice constant of cubic type CdS**)** from TABLE II and 2θ values (compared with JCPDS card number 77-2306) of the samples indicate that cubic type crystal has been formed in all samples for different RF power during sputtering.

A. Effect of RF Power on average crystallite size

Crystallite size has been calculated from the equation as in (5) for all samples fabricated in different RF power from 30 watt to 50 watt and the variations in crystallite size with RF power is presented in Fig.4.

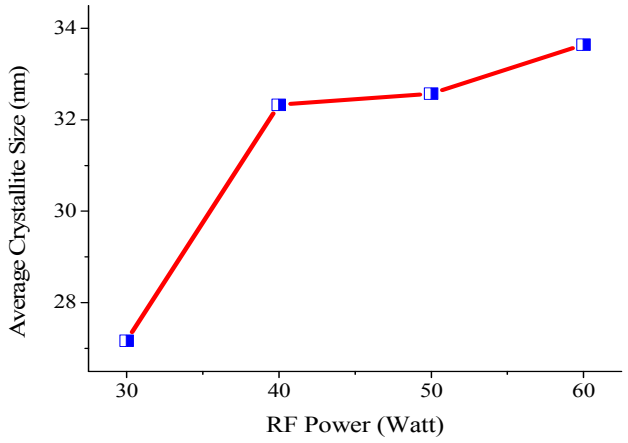

Fig. 4. Crystallite size of as deposited CdS thin-films fabricated at different RF Power

From Fig.4, it is observed that the crystallite size has grown larger with higher RF power. As observed from TABLE I, constant time deposition with varying RF power, film grows thicker for higher RF power due to the incremental linear deposition rate at higher RF power. According to basic physics, crystallite quality improves with higher film thickness as observed from Fig.4.

B. Effect of RF Power on Lattice Constant

Lattice constant for four samples has calculated from the 2θ values and lattice planes of XRD spectra with the help of basic crystal equation and Brag's diffraction equation as in (1) and (4). Calculated lattice constants of four samples deposited in different RF power are shown in Fig.5.

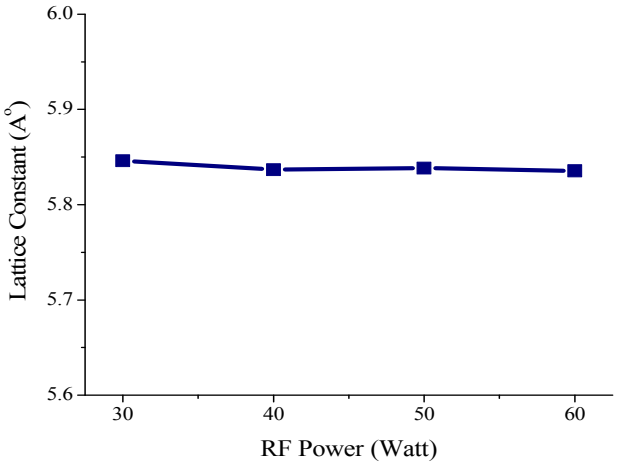

Fig. 5. Lattice constant of RF sputtered CdS films

The figure indicates that lattice constant is fixed for all samples. As lattice constant is a fundamental material property and as deposited material in all samples are cubic type CdS, so the lattice constant for the four samples fabricated at different RF power should be same. The result satisfies the condition, calculated lattice constants for four samples are very close to 5.83 Å (S1:5.84 Å, S2:5.836 Å, S3:5.838 Å and S4:5.835 Å).

C. Effect of sputtering Power on average micro strain

The average developed micro strain in four samples is calculated and its variation with sputtering power is shown in Fig.6.

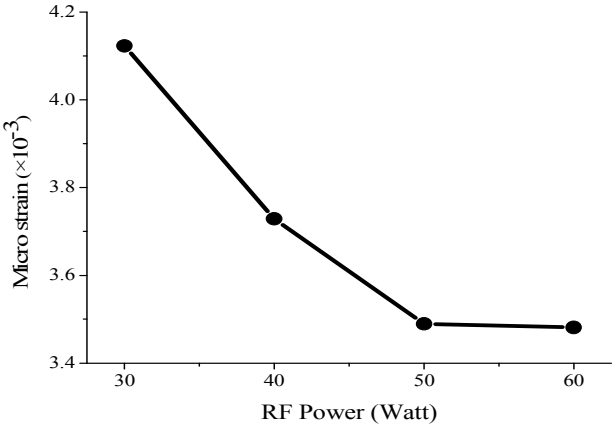

Fig. 6. Micro strain of as deposited CdS thin-films deposited at different RF Power

Film instability results due to the mechanical pressure caused by the differences in lattice constant and thermal extension between the CdS film and SLG substrate. The mechanical pressure causes stress in the films. The stress in the film decreases with higher RF power due to the good crystalline quality of high power deposited films as described in section III. A. After a certain thickness had grown, deposition of CdS was occurred in such a manner that it seems like CdS was deposited on CdS substrate.

D. Effect of RF Power on average dislocation density

Dislocations are caused by the crystal imperfections, differences in lattices in different parts in the crystal. Dislocation lines length per unit volume in crystal is defined as dislocation density. Dislocation density has calculated for four samples and the variation of it with RF power is illustrated in Fig.7.

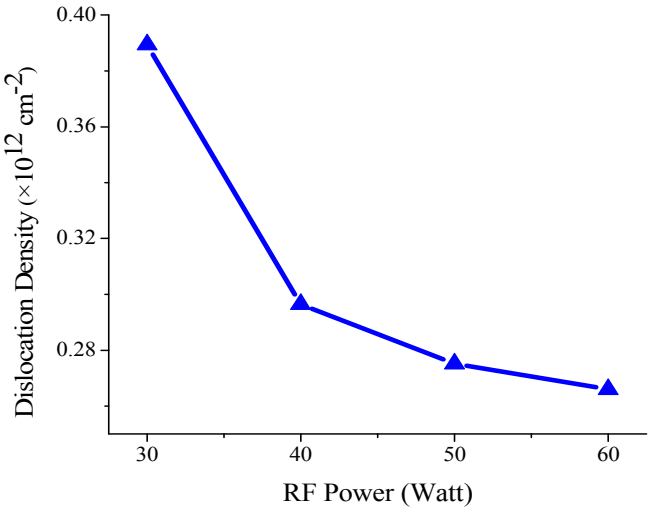

Fig. 7. Dislocation density of as deposited CdS thin-films deposited at different RF Power

From Fig.7, it is observed that the dislocation density has fall for the samples deposited at higher RF power. It is mainly caused due to the reduced strain in samples deposited in higher RF power.

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CONCLUSION

Thin-film CdS has been fabricated on bare soda lime glass substrate by RF magnetron sputtering at different RF power when the substrate temperature was fixed at 100°C for all cases. Deposition rate of CdS has calculated for different RF power and a linear fit was obtained. The XRD data shows that the as deposited films are polycrystalline type in nature and average crystallite size is constant for last three samples (S2, S3 and S4). The microstrain and dislocation density gradually decrease for the high power deposited CdS samples. Also the crystallographic parameters of the deposited films are very close to the literature values [2][3] and high power deposition shows comparatively lower micro strain and dislocation density which can be applicable to form a good heterojunction for thin-film solar cell applications.

REFERENCES

[1] Kevin D. Dobson, Iris Visoly-Fisher, Gary Hodes, David Cahen., "Stability of CdTe/CdS thin-film solar cells*" Solar Energy Materials and Solar Cells*, Volume 62, Issue 3, 15 May 2000, P.p. 295-325

[2] M.A. Islam, M.S. Hossain, M.M. Aliyu, P. Chelvanathan, Q. Huda, M.R. Karim, K. Sopian, N. Amin, "Comparison of Structural and Optical Properties of CdS Thin Films Grown by CSVT, CBD and Sputtering Techniques," *Energy Procedia* 33 (2013), p.p.203 – 213

[3] Sachin Rondiya, AvinashRokade, Adinath Funde, Moses Kartha, Habib Pathan, Sandesh Jadkar, "Synthesis of CdS thinfilms at room temperature by RF-magnetron sputtering and study of its structural, electrical, optical and morphology properties," *Thin Solid Films*, 631 (2017), p.p. 41–49

[4] Miguel A.Contreras, Manuel J.Romero, Bobby To, F.Hasoon, R.Noufi, S.Ward, K.Ramanathan, "Optimization of CBD CdS process in high-efficiency Cu(In,Ga)Se -based solar cells," *Thin Solid Films*, 403 – 404(2002), p.p. 204–211.

[5] A. Ashour, N. El-Kadry, S.A. Mahmoud, "On the electrical and optical properties of CdS films thermally deposited by a modified source," *Thin Solid Films* 269 (1995) 117- 120.

[6] G. Pérez-Hernández, J. Pantoja-Enríquez, B. Escobar-Morales, D. Martinez-Hernández,L.L. Díaz-Flores, C. Ricardez-Jiménez, N.R. Mathews, X. Mathew, "A comparative study of CdS thinfilms deposited by different techniques," *Thin Solid Films* 535 (2013), p.p. 154–157.

[7] A.A.Yadav, M.A.Barote, E.U.Masumdar, "Studies on nanocrystalline cadmium sulphide (CdS) thin films deposited by spray pyrolysis," *Solid State Sciences*, Volume 12, Issue 7, July 2010, Pages 1173-1177.

[8] DavideBarreca, AlbertoGasparotto,CinziaMaragno, Eugenio Tondello, "CVD of Nanosized ZnS and CdS thin films from single-source precursors," *J. Electrochem. Soc*.2004;151(6):G428-35.

[9] Jae-Hyeong Lee , Dong-Jin Lee, "Effects of CdCl2 treatment on the properties of CdS films prepared by r.f. magnetron sputtering," *Thin Solid Films,* 515 (2007), p.p. 6055–6059.

[10] B. S. Moon, J. H. Lee, H. Jung, "Comparative studies of the properties of CdS films deposited on different substrates by R.F. sputtering," *Thin Solid Films*, 511-512 (2006), p.p. 299-303.

[11] Hartmut Frey, Hamid R. Khan, "Hand Book of Thin Film Technology," Springer-Verlag Berlin Heidelberg 2015. DOI 10.1007/978-3-642-05430-3

[12] Eric Lifshin, "X-ray characterization of materials, 37th edt.," WILEY-VCH Verlag GmbH, 1999.