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Characteristics of Cadmium Mercury Telluride Thin Film

S. H. Mane
Department of Physics
Dr. Datar, Behere and Joshi College, Chiplun, Dist- Ratnagiri.
samratmane78@gmail.com, samrat-mane1@rediffmail.com

Abstract: *This paper reports some characterization of polycrystalline cadmium mercury telluride thin film was obtained on ultrasonically cleaned glass substrate in an alkaline medium at 80 ^{0}C by a simple solution growth technique is discussed. The various physical preparative parameters and the deposition conditions such as deposition time and temperature, concentrations of the chemical species, pH, speed of mechanical sturring, etc. were optimized to yield good quality films. The as-prepared sample is tightly adherent to the substrates support, less smooth, diffusely reflecting and was analyzed for composition. The film was polycrystalline with a predominant wurtzite structure. An average crystallite sizes were determined from the XRD patterns and scanning electron microscope (SEM) micrographs. The sample was then characterized optically to determine the absorption coefficient, mode of optical transitions, and the optical band-gap. The surface morphology of this thin film was then observed via a scanning electron microscope. $Cd_{0.9}Hg_{0.1}Te$ crystals are more or less crystalline spherical and hexagonal prismatic in shape. The film shows n-type conduction.*

Keywords: Polycrystalline Thin Film Cadmium Mercury Telluride, Synthesis, Wurtzite Structure

I. INTRODUCTION

Solar energy utilization will play a vital role in solving the world's energy needs of the future [1]. Binaries and pseudo binaries of II-VI and IV-VI group compounds are now becoming focus of intensive research since they exhibit potential as efficient absorber in the visible region of the solar spectrum / 3-5 /. Recently there has been much interest in the application of n-type cadmium chalcogenides, CdX (X= S, Se or Te), electrodes for construction of the photo-electrochemical solar cells / 3-5 /. Among these, CdTe is prominent of all and has ideal matching optical gap and desired n-type conductivity for efficient application in PEC cells [3-5]. Many investigators have pointed out that incorporation of suitable impurities greatly alters the electrical properties of the compound materials. The electrochemical conversion efficiencies of these materials are low and one of the major reasons for such low efficiency is the large resistivity of the electrode material. Therefore, we have concentrated on the investigations of photo-electrochemical properties of the cadmium mercury telluride thin films and to correlate them with their film properties. Further, one of the major factors affecting the quantum conversion efficiency of these photosensitive devices is the form of the photosensitive electrode material. In general, electrodes could be fabricated in different forms: single crystal, thin films, thick films or pellets, etc. Single crystal electrodes are known to yield the highest quantum conversion efficiency for a given material. This is because, amongst the other factors, thickness and the grain boundaries of the material are important parameters influencing the quantum efficiency. Generally, the thickness of the electrode material should be approximately equal to the wavelength of the light corresponding to the band gap of the material. This gives rise to maximum absorption of the incident light without any recombination / 2-7 /. Since the photo sensing properties are direct consequences of the materials characteristics, the choice lies both for the preparation technique and characterization methods.

II. EXPERIMENTAL DETAILS

$Cd_{0.9}Hg_{0.1}Te$ (CMT) thin film was deposited onto the ultrasonically cleaned glass substrates in an aqueous alkaline medium using a simple, convenient, most economical and scalable chemical deposition process reported elsewhere [6-7]. For deposition, cadmium chloride, mercuric chloride and refluxed sodium tellurosulphite (all AR grade) were used as the precursors. Sodium tellurosulphite was obtained by refluxing 4 gm tellurium powder with 90 gm anhydrous sodium sulphite

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in 200 ml double distilled water at 80^0C for 24 hours [6-7]. For deposition of the pure CdTe, 10 ml (1M) $CdCl_2$ solutions was taken in a beaker and 17 ml aqueous ammonia was added to adjust the pH of the reaction mixture (pH = 10 ± 0.2). An appropriate amount of sodium tellurosulphite was then added to the reaction bath. The reaction solution was then made 180 ml by volume. Thoroughly cleaned glass substrates were assembled on a substrate holder and rotated with a constant speed in the reaction mixture to yield the quality films. For the $Cd_{0.9}Hg_{0.1}Te$ films, calculated amount of Hg^{2+} was directly added into the reaction mixture keeping other conditions the same. For quality deposits, time of deposition, the temperature, pH and speed of the substrate rotation were optimized and found to be 90 min., 80^0 C, 10 ± 0.2 and 70 ± 2 rpm, respectively / 6-8/. The structural characterization of the deposited thin films was carried out by X-ray diffraction patterns obtained under Cu-Kα (λ=1.5406 ^{0}A) radiation from a Philips X-ray diffractometer PW-1710. The surface feature of this film structure was therefore examined through a JEOL JSM-6360 scanning electron microscope (SEM), Japan, with an energy dispersive spectroscopy (EDS) technique to measure quantitatively the film composition.

III. RESULTS AND DISCUSSION

An electrolyte is ionically bonded substance, which dissociates in a solvent and increases the ionic conductivity of the solution or acts as a conductor between dissimilar metals in a battery or a galvanic couple. Therefore, an electrolyte match is of importance in PEC cells and it is customary to find out a satisfactory combination of the specific electrode material and an electrolyte. From I-V measurements, it was observed that the higher magnitude of I_{ph} = 157 μA/cm^2 and V_{ph} = 495 mV are obtained for the films deposited at 80 °C and polysulphide (0.25M) electrolyte system offers relatively better match with CdTe and $Cd_{0.9}Hg_{0.1}Te$materials[7-9]. When a light of constant illumination intensity illuminates a PEC cell, the current- voltage characteristic shifts in the fourth quadrant which is in accordance with usual theory of the photovoltaic cell as an electricity generator [2-7,8-13]. The excess charge carriers generated as a result of the photon absorption in the active region of the electrode / electrolyte interface are separated; the electrons move deep into the bulk, while the holes move to the surface of the semiconductor electrode causing redox reactions. The charge separation process continues until it results in a counter field, which is maximum at the open circuit condition called open circuit photo potential.

3.1 The X-ray Diffraction Studies

The X-ray diffractogram was obtained for these as- grown structures in the 2θ range from 20° to 80° to obtain the crystallographic information’s. A representative diffractogram is shown in fig.4. The diffractogram clearly showed that the as -grown film is polycrystalline in nature. The diffractogram was analyzed and the corresponding data (the interplanar distances (d), relative intensities (I/I_{max}), hkl planes, etc.) are presented in table-2 along with the JCPD values. It appeared from the results that pure CdTe and HgTe exhibited hexagonal wurtzite and cubic zinc blende structures [6,14,15]. The strongest reflection of CdTe phase has a d-value of 2.293 A^0 (2.295 A^0 JCPD value), which can be indexed as 110 hexagonal phase. The other dominant reflections of this phase are 101, 103 and their d-values and intensities of reflections follow the similar behavior [10]. A single or two (111, 422) reflections of cubic CdTe have also been detected. The (111) cubic reflection is present and its d-value and intensity of reflection have similar behavior as that of the hex CdTe.

The crystallite size was then determined for the sample using Sherrer’s relation. An average crystallite size was determined from the X- ray diffraction patterns. The average crystallite size (D), wavelength of incident radiation (λ) line width (B) and the diffraction angle (θ) are related as

$$D = k\lambda / B \cos \theta \qquad (1)$$

where k is a constant and is related to the shape of the crystallites, indices of the reflecting planes etc. The value k=0.94 represents the best approximation when little is known about the crystallite size and shape. The determined crystallite size is cited in table 1 .

3.2 Surface Morphology

Micrographs of $Cd_{0.9}Hg_{0.1}Te$ material is shown in fig.5. On addition of Hg in CdTe the surface morphology becomes coarser and changed to spongy or glassy with an orientation towards prismatic and some forms of needle-like structures fused together in a random fashion [6,7,19]. This is the less frequent typical morphology of the hexagonal wurtzite phase of $Cd_{0.9}Hg_{0.1}Te$ occurring mostly in thin layers. It is also pointed out that this typical morphology is a consequence of the growth mechanism that probably, takes place by a diffusion-dislocation mechanism. The observed phase transition (from spherical grannular type cubic to prismatic hexagonal) may be due to the fluctuations in the growth conditions as suggested by Simov et al [16]. In some cases (for higher concentration of Hg), in addition to the increased surface roughness, globules nucleate that tend to agglomerate, resulting in larger sizes. Spallart et al [19] reported similar results. Further, it has been seen that the glass substrate and its crystallographic orientations have no effect on the growth of CdHgTe phases [11,12].

3.3 Optical Absorption Study

The optical absorption spectrum of the $Cd_{0.9}Hg_{0.1}Te$ thin film, corrected for glass substrate absorption, was therefore obtained in the range of wavelengths from 600 nm to 2500 nm. The absorption coefficient of the CdHgTe samples is high, of the order of 10^4 to 10^5 cm^{-1}. In general, the absorption coefficient ($\propto$) and the photon energy (hν) are related as

$$\propto = A(h\nu - E_g)^m / h\nu \qquad (2)$$

where A is a constant and m takes the values 1/2, 2, 3/2 and 3 for allowed direct, allowed indirect, forbidden direct and forbidden indirect transitions, respectively[6,7]. For allowed direct transitions

$$\propto h\nu = A\,(h\nu - E_g)^{1/2}\,. \qquad (3)$$

Thus a plot of $(\propto h\nu)^2$vs hν should be a straight line whose intercept on the energy axis gives the energy gap, E_g [6,7]. Fig. 6. shows the variation of $(\propto h\nu)^2$vs hν for thin film compositions. The estimated band gap of material determined by extrapolating a straight portion of the energy axis at α =1.03 eV. The results are in good agreement with those reported by others [19].

IV. CONCLUSION

The as-deposited samples are polycrystalline in nature and the analysis showed that CdTe exists in the hexagonal wurtzite and cubic zinc blend phases. The surface morphological examination showed a considerable enhancement in the grain structure. The optical absorption studies showed high absorption coefficient with the optical gap 1.03 eV. The mode of optical transitions in these films is of the band-to-band direct type. Thin, uniform, hard, and diffusely reflecting $Cd_{0.9}Hg_{0.1}Te$ film deposition is made feasible by a simple, costless chemical deposition process developed in our laboratory.

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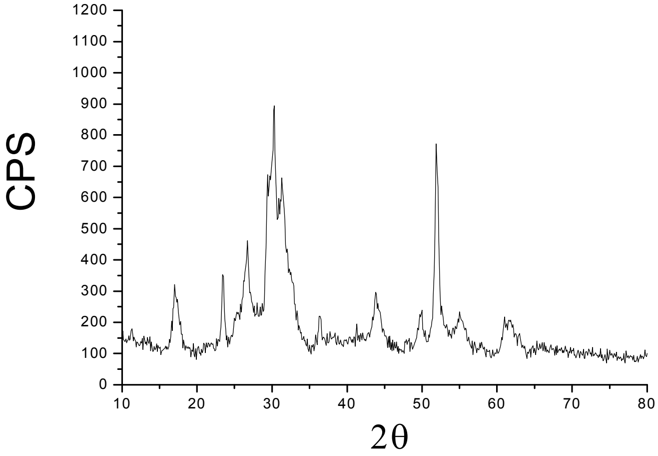

Figure 1: A representative diffractogram of $Cd_{0.9}Hg_{0.1}Te$ photocell

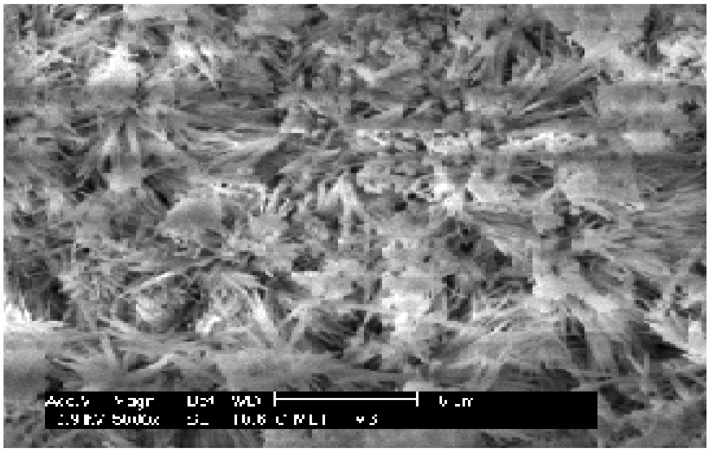

Figure 2: SEM micrograph of $Cd_{0.9}Hg_{0.1}Te$ electrode.

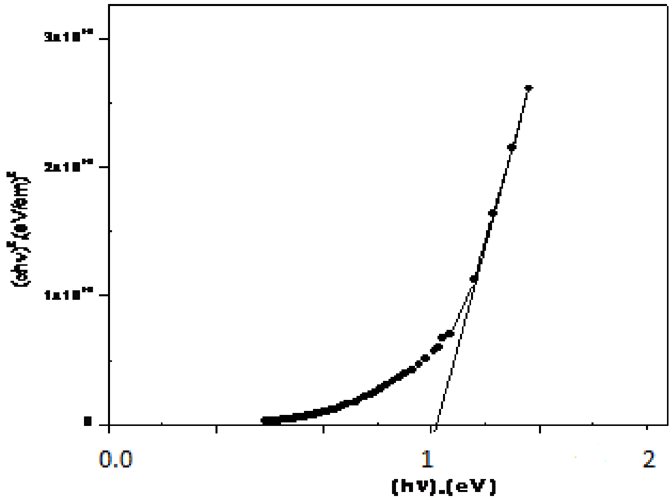

Figure 3: Variation of $(\alpha h\nu)^2$vshν

Table 1: Some parameters of the $Cd_{1-x}Hg_xTe$ thin film

Composition Parameter X	Crystalline size A^0	Crystalline size A^0	Power factor, m
0.1	221	456	0.52

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