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Studies on $CdSe_{0.2}Te_{0.8}$ thin film/(aq) Polysulphide junction photoelectrochemical solar cells

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Abstract:
Thin films of $CdSe_{0.2}Te_{0.8}$ were deposited by vacuum evaporation on highly conducted precoated In_2O_3 glass plates at 300 K at a pressure of 6×10^{-6} torr. The as-grown thin films showed response with (aq) polysulphide electrolyte, (aq) 1 MNaOH + 1 M Na_2S + 1 M S (pH = 12.6) when the junction wasilluminated by white light under AM 1.5illumination condition. The solar power conversion efficiency of the photoelectrochemical (PEC) solar cell was found to be 0.95% . The Mott-Schottky plots in dark showed the flat band potential to be ≈ -1.26 eV*vs SCE*.

1. Introduction:

Thin films of chalcogenides in alloy form mainly Cd-Se-Te have been widely studied for their physical, optical, morphological properties in recent times and solar cell studies. As is studied in the literature [1,2], CdSe exhibits semiconducting properties with hexagonal structure and an optical band gap in the visible spectrum ($E_g \approx 1.72$ eV) and CdTe has an optical band gap of $E_g \approx 1.40$ eV. When an alloy of $CdSe_{0.2}Te_{0.8}$ is synthesized, then new properties are arrived at. In this paper an alloy of $CdSe_{0.2}Te_{0.8}$ in the vacuum evaporated thin film form are characterized for structural studies by X-ray diffraction, optical properties for band gap measurement, potential use of $CdSe_{0.2}Te_{0.8}$thin films in conjunction with (aq) redox polysulphide electrolyte in dark for Mott-Schottky plots and power output characteristics under AM 1.5 white light illumination for efficiency determination of the photoelectrochemical cell.

2. Experimental:

2.1 Preparation of $CdSe_{0.2}Te_{0.8}$

The pure Cd, Se and Te of 99.999 % were taken in quartz ampoule and the ampoule was evacuated in a vacuum of $\approx 6.0 \times 10^{-3}$ torr and sealed. The sealed ampoule was heated in a vertical muffle furnace with constant surrounding temperature of 1200 K for about 8 hours. A uniformly heated homogenous alloy was obtained. The ampoule was gradually cooled to room temperature. The bulk alloy was obtained by breaking the ampoule and grinding it to a finely powdered form in an agate mortar pestle.

2.1 Thermal evaporation of bulk $CdSe_{0.2}Te_{0.8}$alloy and coating of thin films

The thin films of $CdSe_{0.2}Te_{0.8}$of thickness $\approx 400\, nm$ were coated on a pre-coated, conducting Indium Oxide glass plates. The deposition rate of the as-grown thin films was $\approx 3 \pm 1$ nm/s in a vacuum of 6×10^{-5} torr. The substrates were kept at room temperature of

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≈ 300 K. All the as-grown thin films were kept in high vacuum till they were used for preparing photoelectrochemical solar cell device.

2.2. Fabrication of $CdSe_{0.2}Te_{0.8}$/(aq) Polysulphide junction photoelectrochemical cells

A photoelectrochemical solar cell was fabricated using the as-grown $CdSe_{0.2}Te_{0.8}$ /(aq) Polysulphide junction and pure clean graphite as counter electrode. Saturated Calomel electrode (SCE) was used as a reference electrode. The aqueous redox polysulphide electrolytecomprising of AR (analytical reagent) grade chemicals, 1 M NaOH + 1M Na_2S + 1 M S (pH = 12.6) was prepared indoubly distilled deionised water (ρ= 15 $M\Omega$cm).The area of the semiconducting $CdSe_{0.2}Te_{0.8}$with a junction to polysulphide exposed was ≈ 4 cm. White light illumination was performed by SUNLUX (tungsten-halogen) lamp with intensity of 100 mW/cm^2 under AM 1.5 conditions. A capacitance bridge with built in frequency of 1 kHz was used for C-V measurements in dark for generating Mott-Schottky plots.

3. Results and Discussion:

3.1 X-ray diffraction Studies:

As grown thin films of $CdSe_{0.2}Te_{0.8}$ were characterized by powder X-ray diffraction(XRD) method with Ni filter and Cu- $K_\alpha$radiation ($\lambda = 1.542$ Å). The XRD pattern obtained for$CdSe_{0.2}Te_{0.8}$ thin films on bare microslide glass plates was studied in the range of 2θ from 5^o to 80^o. The XRD pattern (Fig. 1) showed that the as grown thin films of $CdSe_{0.2}Te_{0.8}$ were polycrystalline in nature and had a cubic symmetry with a_o= *0.75 nm* [3].

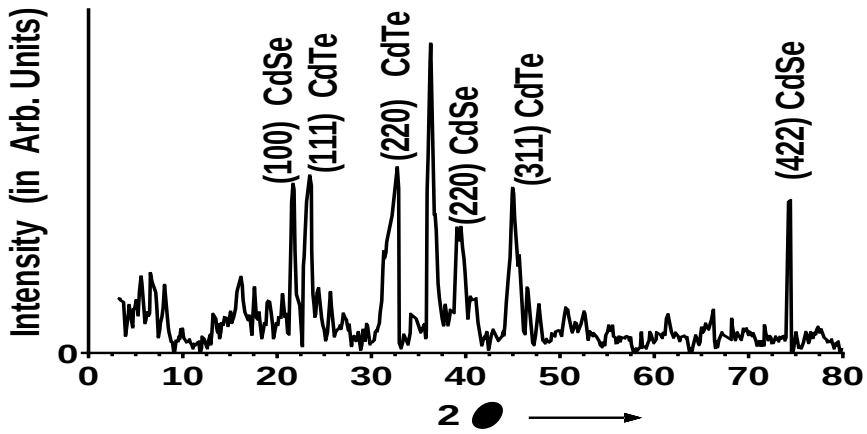

Fig. 1. Powder XRD Pattern of a typical $CdSe_{0.2}Te_{0.8}$ thin film.

3.2Optical Absorption Studies of Thin films for band gap measurement

The thin films of $CdSe_{0.2}Te_{0.8}$ grown over glass plates were subjected to optical absorption studies in the wavelength range of λ= 300 nm to 900 nm.

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For permitted direct transmissions in the optical region the absorption coefficient, α is given by [4]

$$\alpha \approx \frac{A^*}{h\nu}(h\nu - E_g)^{\frac{1}{2}}$$

Where ν is the frequency of incident light, h is the Planck's constant, E_g is the bandgap of the semiconductor and the coefficient, A^* is given by:

$$A^* \approx q^2\left(\frac{2m_e^* m_h^*}{m_e^* + m_h^*}\right)(nch^2 m_e^*)^{-1}$$

Where m_e^* and m_h^* are the effective electron and hole masses respectively, c is the speed of light, h is the Planck's constant and n is the refractive index.

The variation of $(\alpha h\nu)^2$ *vs* $h\nu$ (Fig. 2) gives a straight line plot with intercept on the $h\nu$ axis at $(\alpha h\nu)^2 = 0$ gives the direct optical band gap of the semiconducting $CdSe_{0.2}Te_{0.8}$was around $E_g \approx$ 1.39 eV [5].

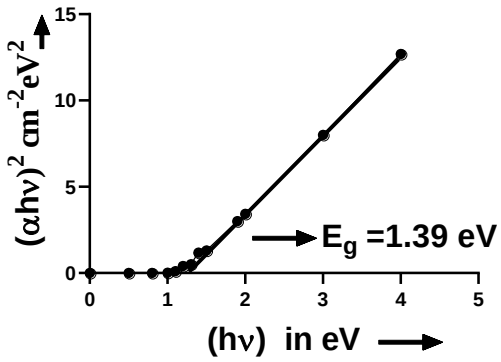

Fig. 2: Plot of $(\alpha h\nu)^2$ *vs* $h\nu$ for a typical $CdSe_{0.2}Te_{0.8}$thin filmgrown over glass

3.3 Mott-Schottky studies of the $CdSe_{0.2}Te_{0.8}$ /(aq) Polysulphide junction

The Capacitance vs Voltage (SCE) were studied for a *$CdSe_{0.2}Te_{0.8}$ /(aq) Polysulphide junction* using a capacitance bridge with built in frequency of 1 kHz in dark. The Mott-Schottky plots were thus obtained for the $1/C^2$ vs Voltage(*vs* SCE) was a linear plot. The intercept of the plot on the Voltage axis for which $1/C^2=0$ is the flat band potential, V_{FB}. The Mott-Schokkty Equation [7,8] is:

$$\frac{1}{C^2} = \left[\frac{2}{\epsilon_o \epsilon_s q N_D}\right]\left[V - V_{FB} - \left(\frac{k_B T}{q}\right)\right]$$

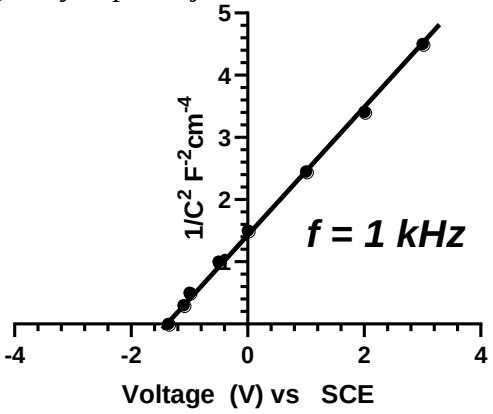

Fig. 3. Mott-Schottky plots in dark for the *$CdSe_{0.2}Te_{0.8}$ /(aq) Polysulphide junction*

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The Flat Band Potential, V_{FB} is given by the condition, $\frac{1}{C^2} = 0$As per our experiment the value of $V_{FB} \approx$ -1.26 eV with respect to SCE.

3.4 Power output Characteristics of the PEC cell.

The power output characteristics of *$CdSe_{0.2}Te_{0.8}$ /(aq) Polysulphide junction*photoelectro-chemical solar cell was studied under AM 1.5 condition under white light illumination. The as grown thin films of semiconducting *$CdSe_{0.2}Te_{0.8}$* showed a power conversion efficiency, $\eta = 0.95$ %. This low value of efficiency is due to the fact that thin film had a lot of defects like small crystallites, many grain boundaries and as grown defects which lead to scattering of minority carriers when the PEC cell is illuminated. These defects also act like recombination centres at the junction itself, thereby reducing the over all power conversion efficiency. Also these as-grown defects contribute to the lower shunt resistance and larger series resistance. This leads to lower fill factor and thus we have low efficiency. There are other reasons like the recombination of charges with the ions of the electrolytes thus preventing these charges to migrate to the external circuit leading to lower conversion of useful solar white light power. Figure 4. shows typical solar power output characteristics of a*$CdSe_{0.2}Te_{0.8}$/Polysulphide photoelectrochemical solar cell* under AM 1.5 conditions. The power conversion efficiency was found to be $\eta \approx 0.95$ % .

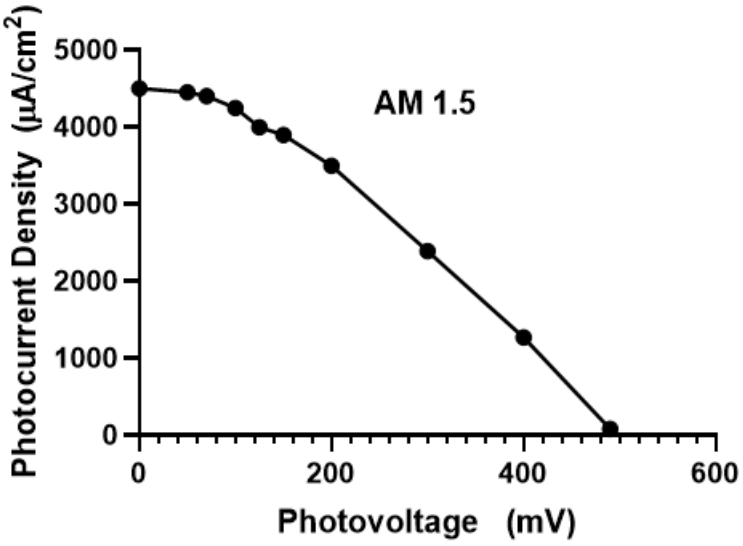

Fig. 4. A typical plot of power output characteristic of a thin film *$CdSe_{0.2}Te_{0.8}$/polysulphide* photoelectrochemical solar cell under AM 1.5 illuminated white light conditions.

4. Conclusions

The as-grown thin films of *$CdSe_{0.2}Te_{0.8}$*were studied for powder X-ray diffraction teachnique. The thin films exhibited polycrystalline nature with d-values matching with literature. The peaks were identified with the literature. From the peaks the thin films showed cubic symmetry due the fact the content of Se was a bit less in the *$CdSe_{0.2}Te_{0.8}$*is evident from the

stoichiometric ratio of Se in the base alloy. The crystalline planes were matched with the literature and the Miller Indices were identified.The optical band gap of as-grown band gap of as grown $CdSe_{0.2}Te_{0.8}$ is $E_g \approx 1.39$ eV which matches with the literature [5]. The Flat Band Potential was found to be V_{FB}= -1.26 V *vs*SCE. This showed that the junction is capable of generating photovoltage. The solar power conversion efficiency was found to be $\eta \approx 0.95$ % . The semiconducting thin films of thin films of $CdSe_{0.2}Te_{0.8}$ had a high potential for use in photoelectrochemical solar cells for power conversion of light to electrical energy. The low solar power conversion efficiency is due to the fact that the as-grown thin film had frozen in defects and small grains thus leading to the fact that there are a large number of grain boundaries which act as scattering centres for the minority carriers generated during the illumination of the semiconductor-electrolyte junction so that the diffusion length is small and thus the power conversion efficiency getting reduced. Also the defects in the as-grown thin films act as recombination centres for the minority carriers near the junctions before the minority carriers do some useful work contributing to the power conversion efficiency. This also leads to high series resistance and low shunt resistance contributing to low fill factor and thus low power conversion efficiency.

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