

Effect of Stainless-steel substrate on $CdSe_{0.4}Te_{0.6}$ thin film/(aq) Polysulphide photo electrochemical solar cell

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Abstract:

Thin films of thickness ≈ 5000 Å of 3% CdSe_{0.4}Te_{0.6} were deposited on stainless steel plates using thermal evaporation in a vacuum of 5×10^{-5} torr on substrates kept at room temperature. Thin films were characterized for powder XRD pattern, showed that zinc blende (Cubic) symmetry with $a_o = 6.295$ Å. The as-grown thin films showed a grain size of ≈ 800 Å. The optical direct band gap of the as grown thin film by optical absorption technique was $\approx 1.419 \ eV$. The solar power conversion efficiency obtained was $\approx 1.25\%$. The results obtained are discussed and analyzed in this paper.

1. Introduction:

Exploring semiconductors in the II-IV group of the periodic table, it was found that other Si and Ge there are other elements which show semiconducting properties like an alloy mixture of Cd-Se-Te where the band is direct one and the band gap of such alloys lie in the visible spectrum of the solar energy as received on the surface of the earth. These materials in solid bulk form have been explored earlier. However, there is a large scope of use of these materials in the thin film form where the application of solar cells as far as solar cells is concerned. A photo electrochemical solar cell with of stainless-steel substrate based CdSe_{0.4}Te_{0.6} with junction of polysuphide shows a promising result. The effect of the stainless-steel substrate on which a thin film is grown and used for fabrication of photo electrochemical solar cell is discussed here.

2. Experimental:

Bulk solid Cadmium, Selenium and Tellurium with high purity of 99.999% were used to make an alloy at 580 °C in a vacuum sealed quartz ampoule placed in a muffle furnace which was heated for 12 hours. The muffle furnace was gradually cooled step by step of 5 °C per minute to room temperature. The ampoule was cooled and its end was crushed to get a homogenous bulk alloy. This alloy was cleaned in ethanol and ground in an agate mortar pestle till a fine powder was obtained. A Tantalum boat was used to evaporate inside the vacuum system at a pressure of $\approx 5 \times 10^{-5}$ torr by passing a current of 2 A for 54 seconds. A thoroughly pre-cleaned Duplex Stainless steel plates were used as a substrate to coat the thin films at room temperature. A quartz crystal monitor was used to monitor the thickness to obtain the desired thickness of the thin film. Experimental samples were kept in high vacuum so that the surface of the thin film doesn't combine with ambient oxygen to form an oxide layer. A redox electrolyte, viz., Polysulphideelectrolye made of (aq) 1 M Na₂S + 1 S + 1 M NaOH was used in conjunction with the semiconducting thin film and a graphite counter electrode was used to make a photo electrochemical solar cell. A double distilled water was used to make the electrolyte. A tungsten-halogen lamp was used to illuminate the photo electrochemical solar cell with an illumination intensity of 100 mW/m2 was used to realize AM 1.5 conditions in the laboratory. The XRD studies were done with CuK_{α}



radiation to know the crystal structure of the thin film. UV-VIS-IR spectrophotometer was used to study optical absorption and ascertain the band gap.

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3.1 X-ray diffraction analysis of $CdSe_{0.4}Te_{0.6}$ alloy, bare stainless steel plates and $CdSe_{0.4}Te_{0.6}$ grown over stainless steel plates

The as-grown thin films of $CdSe_{0.4}Te_{0.6}$ on stainless steel substrates were subjected to powder X-ray diffraction. The X-ray diffraction of the bulk powder of $CdSe_{0.4}Te_{0.6}$ was also studied. The X-ray diffraction pattern of the bare stainless-steel plate was also studied. It is seen that the stainless-steel shows prominent peaks corresponding to α - steel, γ - steel in our samples. The peaks of our stainless-steel samples matched with those of the literature [4]. The h,k,l values of the bulk powder matched with those of literature. Also, there some peaks missing in the thin film due to preferential orientation of the grains in the as-grown thin films. As usual the thin films grown on stainless substrates showed peaks of stainless steel as well as those of the semiconducting material. It is found that the from the XRD studies the thin film exhibited Zinc Blende structure with cubic symmetry [5] with lattice constant, $a_0 \approx 6.316$ Å. Figure 1. shows a typical X-ray diffraction pattern for bare stainless steel thin film, bulk powder and as-grown thin film.



CdSe_{0.4}Te_{0.6} thin film on stainless steel substrate

3.2 Optical absorption studies of the $CdSe_{0.4}Te_{0.6}$ alloy thin films

The as-grown thin films were studied by means of a tauc plot. The experimental data for the optical properties of the as-grown thin films of $CdSe_{0.4}Te_{0.6}$ were subjected to optical absorption in UV-VIS-IR region for optical band gap studies. On obtaining the values of optical absorption coefficient, α for each wavelength, λ the corresponding energy, hv was calculated. For permitted direct transmissions in the optical region the absorption coefficient, α is given by [7]

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

Where $\boldsymbol{\nu}$ 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:



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

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 $(\alpha hv)^2 vs hv$ (Fig. 2)gives a straight line plot with intercept on the hv axis at $(\alpha hv)^2 = 0$ gives the direct optical band gap of the semiconducting CdSe_{0.4}Te_{0.6} was around E_g^{\approx} 1.419 eV.



Fig. 2. A plot of $(\alpha hv)^2 vs (hv)$ for an as grown $CdSe_{0.4}Te_{0.6}$ thin film on stainless steel substrate.

3.4 Solar Power conversion studies for the as-grown $CdSe_{0.4}Te_{0.6}$ alloy thin film/polysulphide junction photo electrochemical solar cell

The solar power conversion efficiency was studied for the as-grown $CdSe_{0.4}Te_{0.6}$ alloy thin film/poly sulphide junction photo electrochemical solar cell. The Current density vs Photo voltage characteristics [8-9] were obtained as shown in the Fig. 3. It is seen that the fill factor as obtained as FF \approx 35%, Open Circuit Voltage, $V_{OC} \approx 0.56$ V and the short circuit current density, $J_{SC} \approx 4500 \,\mu$ A/cm², this is due to the fact that the as-grown thin films exhibit frozen-in defects during the growth of the thin film as the evaporating material gets deposited. This deposition can have agglomeration and defects in the thin film. It is due to these defects there is a lot of surface scattering of the minority charge carriers on illumination at the semiconductor electrolyte junction. Thus, the efficiency and fill factor are found to be low. The solar power conversion efficiency is \approx 1.25%. Figure 3 shows a typical plot of solar power output characteristics of photo electrochemical cell.





4. Conclusions

The semiconducting $CdSe_{0.4}Te_{0.6}$ alloy in thin film form shows a promising property of solar power conversion when a junction of $CdSe_{0.4}Te_{0.6}$ alloy thin and polysulphide is made. Also substrate material like highly conducting stainless steel when used can be a promising substrate material. The properties of $CdSe_{0.4}Te_{0.6}$ alloy on stainless steel exhibit their characteristic nature. The XRD studies show that $CdSe_{0.4}Te_{0.6}$ alloy has Zinc Blende cubic symmetry with lattice constant matching fairly with the literature. Also, the optical absorption studies too show a remarkable closeness to the direct band gap nature with $E_g \approx 1.419$ eV. The solar power conversion efficiency studies at AM 1.5 illumination have shown that the photo electrochemical solar cell exhibits a solar power conversion efficiency of 1.25 %.

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