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Preparation, characterization and *ab-initio* study of $CdSnTe_2$ thin films by closed space sublimation technique

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ABSTRACT

The cadmium tin telluride (CdSnTe) alloy was prepared by direct reaction of high purity elemental constituents using rotating furnace. Thin films of CdSnTe different thickness were prepared on glass substrates by vacuum closed space sublimation method. The films were subjected to XRD, SEM, EDAX and UV–vis–NIR studies. The crystalline structure of CdSnTe alloy was found to be face-centered cubic with lattice parameter 6.30 Å. EDAX studies confirmed the composition of the alloy as $CdSnTe_2$ compound. The UV–vis–NIR optical transmission spectra of thin films of different substrate temperatures were obtained. The energy band gap found to be in the order of 1.5 eV. The band gap is suitable for LEDs, optoelectronics and photovoltaic applications. First principle density functional theory calculations of $CdSnTe_2$ structure were performed by using Vienna *ab-initio* simulation package software. The results of theoretical calculations are in good agreement with experimental data.

1. Introduction

Industrialization and urbanization demands more and more electrical energy. Technological advancements are reducing the cost of electrical energy production by utilizing solar energy. Solar energy is sustainable and a non-polluting renewable source of energy. The world wide support for photovoltaic conversion increases and the production of photovoltaic modules grows exponentially [1–4]. The direct band gap CdTe cells with high optical absorption coefficient are cost efficient, stable and suitable for photovoltaic applications [5–9]. Band gap of CdTe is around 1.5 eV [10–12]. The efficiency of CdTe solar cells are above 16% [13,14]. Recently, ternary and quaternary compound semiconductors are attracting more attention due to tunable band gap [15,16]. Sn-doping to CdTe results in the CdSnTe formation. Sn enhances conductivity whose absorption coefficient is more than CdTe. CdSnTe is a ternary compound which finds suitable for LEDs. photovoltaics and optoelectronic sensors [17–19].

Thin films of CdTe-related compounds can be deposited by different methods [20,21]. Besides thin film deposition, this technique was widely applied for the high-quality crystal growth of volatile compounds [22,23]. Closed space sublimation method is the suitable technique for the deposition of high efficiency solar cells at high substrate temperature (600–900 K) and this technique has been adopted by many researchers for the CdTe-based thin film deposition [24–29]. The experimental set up having a closed bottom end quartz tube containing the alloy at bottom is heated using tungsten wire wound in the form

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of boat. The films to be coated on the glass substrate is made to rest over the quartz tube separated by a distance using a horizontal copper disc supported by a vertical shaft fixed to the slow speed DC motor. The copper circular disc has 8 circular slots in rectangular cavities and this provides a capability to fabricate eight films with variable thickness simultaneously under same conditions. Fig. 1 shows the specially designed closed space sublimation unit fabricated for the deposition of CdSnTe thin films. The whole set up is covered by a semi-cylindrical glass jar to deposit the thin films in vacuum. Sublimation of the alloy from the quartz tube on to the glass substrate takes place when the quartz tube is heated by the tungsten boat connected to 220 V AC power supply with variable output current. The temperature of the source and substrate were measured and controlled by chromel–alumel thermocouple with the accuracy of 1 °C.

2. Experimental details

2.1. Preparation of CdSnTe thin films

High purity elements Cd, Sn and Te (99.999%, Sigma Aldrich) were used for the bulk alloy preparation. Stoichiometric mixture of cadmium, tin and tellurium needed for the preparation of $CdSnTe_2$ alloy was inserted in to the quartz ampoule of 8 cm length and 1 cm diameter. The pressure inside the quartz ampoule was reduced to 10^{-4} Torr and evacuated to vacuum condition using a vacuum chamber. The quartz ampoule was heated gradually to 1000 K at the rate of 100 K per hour for a period of 6 h using rotating furnace (15 rpm). The ampoule rotation during heating ensures mixture homogenization. The reacted mixture was cooled to room temperature at the rate of 100 K/h. The prepared alloy was preserved for thin film deposition. The $CdSnTe_2$ charge of 1 mg was taken in a clean quartz tube with narrowed closed end of size 1 cm diameter and 1.5 cm height and placed in the tungsten boat present in closed space sublimation unit. The cleaned glass substrates of 25×37.5 mm^2 in size were carefully placed in the rectangular cavities with circular slots in the copper disc mounted just above the open end of the quartz tube at a distance of 5 mm. The entire set up was covered with glass jar having rubber gasket so as to deposit the thin films in vacuum condition. The pressure inside the set up was reduced to 10^{-5} Torr using a combined unit of diffusion pump backed by rotary pump. The source heater (tungsten boat) was heated gradually using power supply followed by rotation of circular disc slowly with the help of slow speed motor. The alloy vaporization takes place between 500 K and 1100 K. The temperature of the glass substrates were raised to 400 K at the time of deposition. The procedure was followed by changing the substrate temperature to 500 K and 600 K. The prepared thin films were preserved for characterization.

The film thickness was estimated using a multiple beam interferometer. X-ray diffractometer (JDX 8030) with Ni filter under 2θ scan coupling mode with 40 KV and 30 mA current ratings was used to confirm the structural properties of $CdSnTe_2$ thin films. EDAX measurement (JOEL 6390) was done to estimate the bulk composition of the films. The optical properties were studied using spectrophotometer (JASCO-370V).

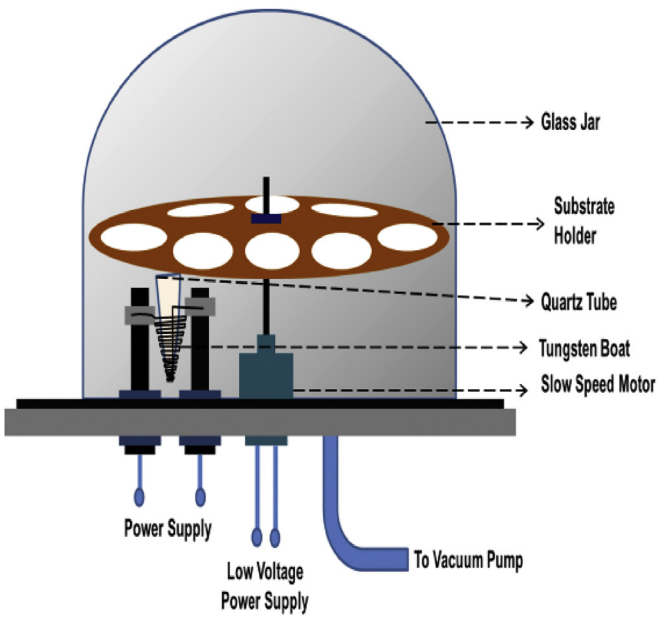

Fig. 1. Closed space sublimation unit.