Characterization of vacuum flash evaporated CdTe thin films for solar cell application

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Abstract. This paper reports the results of CdTe thin films characteristics deposited by vacuum flash evaporation technique. The characteristics of CdTe films deposited at different substrate and evaporator temperatures were analysed using different methods. XRD results have shown that all samples exhibit a predominant sharp peak at 2θ around 23.80 which is assigned to the (111) plane of zinc blend cubic structure. AFM images of CdTe thin films have shown that grain size increases with increasing the substrate temperature, which correlates with XRD results. We have found that the decrease the evaporation temperature from 850°C to 650°C leads to the drastically increasing of the average grains sizes from 60 nm to 600 nm. The transmission and reflection spectrum of CdTe thin films are used to evaluate the bandgap Eg. All films have Eg (1.49 eV - 1.50 eV) correspond to the bandgap of a bulk CdTe crystal.

1. Introduction
In last decade cadmium telluride (CdTe) is of great interest as one of the most promising material for low cost and effective solar cells application [1]. CdTe has been considered as one of the most attractive semiconductor absorber layer in thin film solar cells due to its optimal direct bandgap 1.5 eV and high (more than 5·10⁵ cm⁻¹) absorption coefficient. A theoretical limit of one-junction CdTe solar cells is more than 30% for AM1.5. [1]

Characteristics of CdTe thin films strongly depend on the applied deposition technique. Various techniques have been reported for deposition of CdTe thin films such as physical vacuum deposition [2], electro deposition [3], closed-space sublimation (CSS) [4] and etc. The highest published in scientific journals efficiency of 16.5% is obtained by using CSS technology [5]. In spite of high value of efficiency, the main disadvantage of CSS technology is the high (650-700°C) temperature of the process, additionally requires expensive special heat-resistant glass substrates [6]. That is why the further development of low temperature methods of CdTe layers deposition is important not only from standpoint of reducing the power consumption, but also for production of solar cells on flexible polymer substrates.

Among the low temperature techniques for manufacturing CdTe solar cells the most suitable are the magnetron spattering [7, 8] and physical vacuum evaporation techniques [9]. The best results were obtained by the method of vacuum thermal evaporation. However, by means of this technique it is difficult to deposit the films of II-VI compounds of strictly stoichiometric composition. From this point of view is more acceptable the flash evaporation technique which is the variation of the thermal vacuum evaporation. Despite this technology advantages there is a limited number of works dedicated to application of this technique for deposition of chalcogenide thin films [10, 11].

As it is described in work [11] the stoichiometric composition of chalcogenide films is achieved because the deposition is performed by discrete evaporation of small portions of alloy to be deposited.
Small particles of crushed chalcogenide alloy whose constituents have different partial vapor pressure fall down into the preheated flash exchanger. Since the particles have different sizes and fall down in a random way at each moment in the flash exchanger there are some amounts of particles which have different temperatures and are at different evaporation stages. Due to the simultaneous presence of such particles in the flash exchanger the composition of deposited film repeats the stoichiometric composition of evaporated material.

In this work, we for the first-time applied vacuum flash evaporation technique to deposit CdTe thin films on glass substrate and investigated the substrate and evaporator temperature’s influence on the structural, morphological and optical characteristics of CdTe films which act as an absorbing layer in chalcogenide solar cells.

2. Experimental details
Thin films of CdTe were fabricated by flash evaporation technique on glass substrate with thickness 1 mm and diameter 20 mm, which were cleaned by standard semiconductor technology methods.

The source material was CdTe crystals (99.999%) crushed to a powder with particle size of 50 μm – 150 μm. The vacuum chamber before evaporation was pumped to a base pressure of 1.5 × 10^{-5} Torr. Dispensing the CdTe particles from batcher onto the molybdenum flash exchanger was performed due to opening and closing of batcher outlet [11].

Thickness of CdTe films and their deposition time were 1 - 2 μm and 30 - 50 min, respectively.

3. Results and Discussion
3.1. Structural analysis of CdTe thin films
Figure 1 shows the X-ray diffraction patterns of CdTe thin films recorded over 2θ range from 15° to 70° with the step 0.1°. All CdTe films deposited at 100°C, 175°C and 250°C substrate temperatures exhibit a predominant sharp peak at 2θ around 23.8° which is assigned to the (111) plane of zinc blend cubic structure [ASTM x-ray powder data file, card No. 15-770]. These diffraction patterns show that the (111) orientation increases while decreasing the process temperature, and the results are in good agreement with the same results observed in [12]. The average grain sizes (D) of the film was calculated using the Scherrer’s equation [13].

![Figure 1. XRD patterns of CdTe films deposited at substrate temperature: a) 100°C, b) 175°C, c) 250°C](image)

The grain size varies with increase the substrate temperature non-monotonically. At first with the temperature increase from 100°C to 175°C the grain size decreases from 53.9 nm to 42.1 nm then from 175°C to 250°C increases from 42.1 nm to 57.4 nm.
3.2. Optical analysis of CdTe thin films

The results of optical measurements of CdTe thin films deposited at different substrate temperatures are presented in Figure 2 and Figure 3.

![Figure 2](image2.png)

**Figure 2.** The plot of absorption coefficient ($\alpha$) vs. photon energy ($\hbar\omega$) at 100°C, 175°C and 250°C substrate temperatures.

The optical bandgap, $B$ is a constant. Using this equation, the value of CdTe thin films optical bandgap have been calculated and were determined to be 1.50 eV, 1.49 eV and 1.49 eV at substrate temperatures 100°C, 175°C and 250°C, accordingly. The thin film of CdTe deposited at 100°C has the same optical bandgap as the CdTe bulk crystal.

![Figure 3](image3.png)

**Figure 3.** Plots of $(\alpha \cdot \hbar\omega)^2$ vs. photon energy ($\hbar\omega$) at 100°C, 175°C and 250°C substrate temperatures.

3.3. Surface morphology of CdTe thin films, deposited at different substrate and evaporated temperatures

Figure 4 shows typical 2μm x 2μm AFM images and grain size bar chart of CdTe films deposited on a glass substrate at 250°C and at evaporator temperature 800°C-850°C. The AFM images of films, deposited on substrates having different temperatures showed that substrate temperature increase from 100°C to 250°C leads to only a small increase in grain size (the biggest grain size increased from 120 nm to 160 nm, about 30%). These results are in good agreement with the average grain sizes calculated from XRD results.

![Figure 4](image4.png)

**Figure 4.** AFM images and the grain size bar chart of CdTe thin films, deposited on substrate at 250°C.

In experiments we have observed, that the grain size depends also on the evaporator temperature. We have found that the grains of huge size (in average 600 nm) are resulting from evaporator temperature
(600°C-650°C) and at substrate temperature 250°C. For comparison, the best results of CdTe thin films deposited by thermal vacuum evaporation technique had the grain sizes of about 100 nm [15]. The AFM images of these films surface morphology and grain size distribution are shown in Figure 5. The XRD results show, that CdTe films deposited at these technological conditions have the best crystalline structure.

![AFM images and the distribution of grain sizes of CdTe thin films, deposited at evaporator temperature 600°C. The substrate temperature was 250°C.](image)

**Figure 5.** AFM images and the distribution of grain sizes of CdTe thin films, deposited at evaporator temperature 600°C. The substrate temperature was 250°C.

**Acknowledgments**

The authors are thankful to the Ministry of Education of the Russian Federation for providing financial assistance of this research, as well as to the Competitiveness Program of National Research Nuclear University MEPhI, for organization of conference and publication of its proceedings.

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