# Structural and optical properties of CdTe solar cell films at different substrate temperatures

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Solar cell absorption layer based on CdTe films were successfully deposited at various substrate heating processes (25, 200 and 400 ℃) by magnetron RF-sputtering. The film structures, morphologies, and optical properties had been characterized by X-ray diffraction (XRD), atomic force microscopy (AFM) and US spectrophotometer. The XRD study revealed that CdTe film at 200 ℃ exhibited cubic and hexagonal structures while single cubic structure appeared at room temperature and 400 ℃. Moreover, the AFM result showed that the structure shapes and grain sizes were slightly different in the films at various substrate temperatures. Finally, the optical measurements suggested that the CdTe film at 200 ℃ showed better optical behavior than other films.

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*Keywords:* Thin film, CdTe, Substrate heating processes, Vapor deposition, Optical properties

CdTe is a II-VI compound semiconductor which has been used in several optoelectronic devices such as solar cells and radiation detectors. The energy of its band gap of 1.5 eV, located at the maximum of the solar energy density incident on the earch surface, makes this material very suitable for photovoltaic applications [1, 2]. Besides, CdTe films possess certain exceptional material characteristics including band-gap, absorption coefficient and minority carrier diffusion length which are particularly suitable for photovoltaic applications [3, 4].

Various techniques such as RF-.sputtering [5], spray pyrolysis [6], co-evaporation [7], chemical bath deposition [8] and electrodeposition [9, 10] have been used to fabricate CdTe thin films. Each technique has its own merits, but from the point of view of the film performance, the RF-.sputtering seems to be best suited [11, 12]. It is well known that properties of CdTe films are strongly dependent on the preparation methods and deposition parameters [13, 14] due to obtained stoichiometry and microstructure. For this reason, it is essential to characterize their properties according to the deposition parameters.

During the last few years, considerable efforts have gone into optimization of the thin film quality, whereas much less has gone into the phase change and optical properties of CdTe films. In this work, it is presented the influence of the sputtering parameters such as substrate temperatures on the structures and optical properties of CdTe films. The acquired results and related discussions would be feasible for their potential applications.

## 1. Experiment

### 1.1 Synthesis of CdTe thin films

A CdS film layer was deposited firstly on the SFO ($SnO_2$: F) glasses used a power of 50 W, and then the CdTe absorbed layer was prepared at power of 100W on the CdS films. Thin films of CdTe and CdS were all deposited by RF-sputtering using magnetron sputtering system (FJL560D2). The cylindrical CdTe (Cd: Te = 1:1) and CdS ceramic targets of 8 cm diameter were used. No changes in target composition were observed with time and usage. The deposition chamber's base pressure was $1.6\times10^{-4}$ Pa, and during deposition the gas pressures were maintained constant at 0.5 Pa. The substrate-to-target distance was 100 mm. Depositions of CdTe and CdS layer were performed for 180 and 25min, respectively. Finally, all the samples were deposited at various substrate heating temperatures (25, 200 and 400 ℃). The process parameters of CdTe films used in RF magnetron sputtering are shown in Table 1.

*Table 1. Sputtering parameters of CdTe films.*

| Sample | Sputtering pressure /(Pa) | Sputtering power / (W) | Sputtering temperature / (℃) |
|---|---|---|---|
| a | 0.5 | 100 | 25 |
| b | 0.5 | 100 | 200 |
| C | 0.5 | 100 | 400 |

### 1.2 Characterizations of CdTe films

Optical properties of the CdTe films were measured at normal incidence using a double-beam ultraviolet–visible–near-infrared spectrophotometer (Shimadzu) with optical transmittance in the photon energy range of 1.1-6.6 eV. To investigate crystallographic properties of the films, coupled θ-2θ X-ray diffraction (XRD) scans in the film mode were performed in the range of 2θ=20$^o$-80$^o$ by use of the Cu Kα1 line of the X-ray source (Rigaku D/max2550). The surface morphologies of films were examined by atomic force microscopy (DI Nano-scope ⅢA Multimode).

## 2. Results and discussion

### 2.1 Structural studies of CdTe films

Fig. 1 shows the XRD patterns of CdTe films deposited at different substrate temperatures by magnetron RF- sputtering. It is observed in Fig. 1 that two structures phase occurred in 200 ℃ film. The zincblende (cubic) structure is mainly confirmed by the (1 1 1), (2 2 0) and （3 1 1) diffraction peaks at 2 theta = 23.6◦, 39.2◦ and 46.4◦, which followed by a wurtzite (hexagonal) structure confirmed by (0 0 2) peaks at 2 theta = 22◦ [15]. However, the intensities of the (1 1 1), (2 2 0) and （3 1 1) peaks were extremely high in comparison with the (1 1 1) one. This indicates a preferential orientation of the micro-crystallites with the (1 1 1) direction perpendicular to the substrate at 200 ℃.

When the substrate temperature (room temperature and 400 ℃) are used to deposition, only three characteristic peaks (1 1 1), (2 2 0) and （3 1 1) are displayed in these samples, indicating that single phase (cubic structure) appeared in these films. Increasing the suitable substrate temperatures cause the phase formation from the cubic structure to the hexagonal structure. This result may be due to the fact that in the room temperature and 400 ℃deposited CdTe films no additional tellurium is supplied and the diffusion of Te is not enough to the formation of stiochiometric CdTe [16].

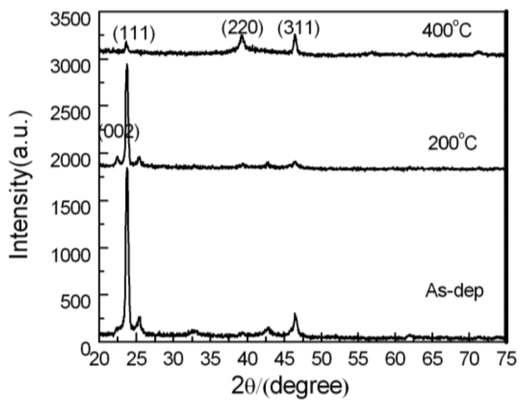


*Fig. 1. XRD patterns of CdTe films deposited at various substrate temperature.*

### 2.2 Morphological studies of CdTe films

Fig. 2 (a-c) shows the AFM images of the CdTe films deposited on different electrodes. The images were measured with a scanning area of 10 μm. It can be found in Fig. 2 (a) that the CdTe film deposited at room temperature has some anisometric particles, which have a well-defined shape and relatively uniform size. Also, some pin holes and voids can be observed in the film at room temperature. It could be attributed to the large number of lattice mismatch and defects in the growth stage of CdTe film.

It can be seen in Fig. 2 (b) that the film seems to expose very compact morphologies with fewer pin holes and voids. It can be due to the complete diffusion of the atoms when the enough kinetic energy can be supplied to the atoms at the increasing substrate temperature. Also, the size of the crystalline grain deposited at 200 ℃ is larger than that at room temperature. Obviously, the suitable substrate heating treatment (200 ℃) can improve the growth condition to reconstruction of the crystal.

It can be found in Fig. 2 (c) that the large grains with well defined grain boundaries and some big cracks appear in the CdTe films at 400 ℃. It is clear that the higher substrate heating treatment has a significant effect on the regrowth and recrystallisation of the CdTe grains. However, the thermal stress arising form the difference of expansion coefficient of the film and substrate can lead to the aggregates of the cracks.

### 2.3 Surface roughnesses and grain diameters of CdTe films

Table 2 summarizes the data of grain size and film thickness resulted from Fig. 2 (a-c). It can be seen from Tab.2 that the films became rougher when the substrate temperature increased from 200 ℃to 400 ℃. Additionally, a comparison between the micrograph (c) and the previous micrographs (a-b) reveal clearly a significant increase in the average grain size of the film (400 ℃) and apparition of pinholes as well.

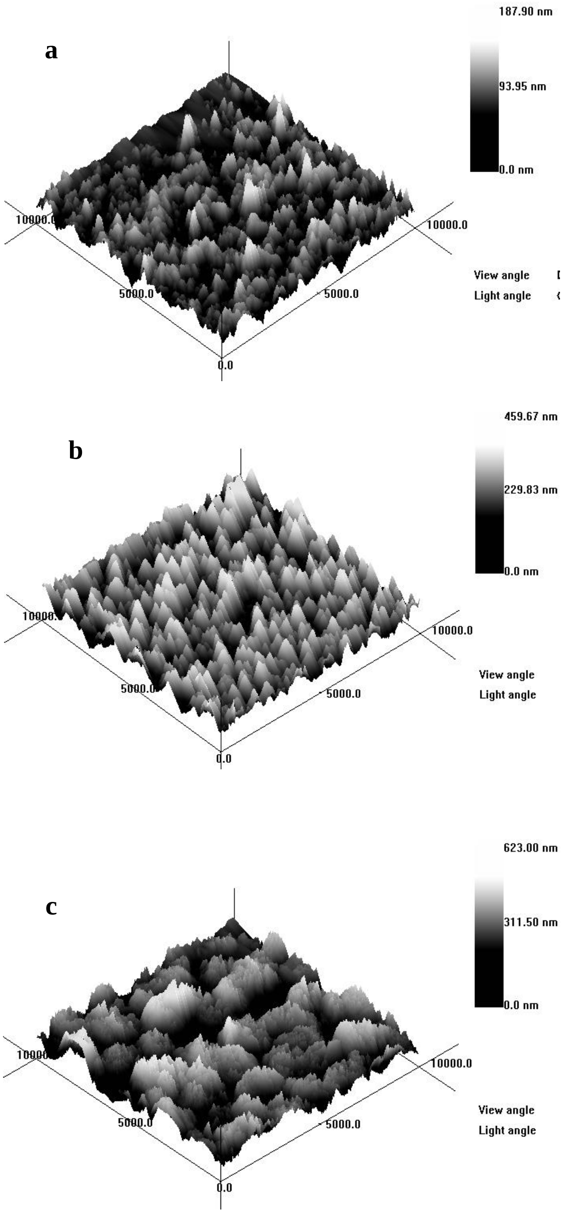


*Fig. 2. AFM images of cross sections CdTe films deposited at various substrate temperature.*

*Table 2. Surface rougnesses and grain diameters of CdTe films.*

| Sample | Sputtering temperature / (℃) | Dimeter / (nm) | Roug-nesses /(nm) |
|---|---|---|---|
| a | 25 | 114.78 | 30.34 |
| b | 200 | 186.14 | 43.21 |
| C | 400 | 813.99 | 78.39 |

### 2.4 Optical properties of CdTe films

Fig. 4 shows the spectra curves of CdTe films on different substrate temperatures in the wavelength range 200-1100 nm. It can be found in Fig. 4 that the optical transmittance spectra of the films at 200 and 400 ℃ exhibit good transmissions in the visible region compared with the film at room temperature. It indicates that the improved transmittance is associated with the enhanced crystallinity of the CdTe films in the substrate heating treatment.

Moreover, it can be found that the optical transmittances of the CdTe films in all samples are slightly degraded in the 600-800 nm range and that of film at 200 ℃ was fastest. This means that the film at 200 ℃ has a best absorbance to in visible light domains (600-800 nm). It indicates the uniform film in the suitable substrate heating treatment reduces the loss of light due to scattering and results in the increase in the absorbance.

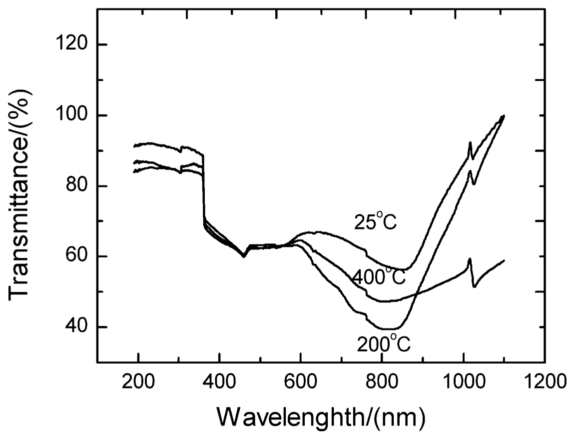


*Fig. 3. Transmittance spectra curves of CdTe films deposited at various substrate temperature.*

## 3. Conclusions

1) The XRD patterns show that the CdTe film at 200 ℃ was found to exhibit cubic and hexagonal structures while that at room temperature and 400 ℃ appear single cubic structure. It may be due to the reason that no additional tellurium is supplied and the diffusion of Te is not enough.

2) The result of AFM morphologies indicated that the increase of the grain size and the decrease of the defects can be seen in the film at the suitable substrate heating treatment (200 ℃). However, the large grains with well defined grain boundaries and some big cracks appear in the films at 400 ℃.

3) The optical transmittance spectra suggest that the CdTe film at 200 ℃ exhibit better absorbance to in visible light domains (600-800 nm) than the other films. It is concluded that the improved transmittance is associated with the enhanced crystallinity of the CdTe films in the substrate heating treatment.

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