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Influence of substrate temperatures on morphologies and optical properties of CdTe solar cell films

XIN JI [*], LIN JUN WANG, JIAN YONG TENG, YI MING MI[a], CHAO MIN ZHANG[a]
School of Materials Science & Engineering, Shanghai University, Shanghai 200444, China
[a]*College of Fundamental Studies, Shanghai University of Engineering Science, Shanghai 201620, China*

Solar cell absorbing layer based on CdTe films were successfully deposited by magnetron RF-sputtering with different substrate temperatures (25, 200 and 400 ℃). The effect of substrate heating processes on the film surface morphologies, section morphologies and optical properties was investigated in detail. The surface morphologies results show that the increase of substrate temperature is in favor to change the grain size and structure shape. The section morphologies results implied the density of grains was increased with increasing grain sizes when substrate temperature increased from 25 to 200 ℃. Furthermore, it is indicated that 200℃ is the best substrate heating process in the optical properties in the all samples.

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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 morphologies and optical properties of CdTe films. In this work, it is presented the influence of the sputtering parameters such as substrate temperatures on the morphologies 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 1.6×10^{-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 absorption in the photon energy range of 1.1-6.6 eV. The surface and cross-section morphologies of films were examined by scanning electron microscopy (SEM-3400-N).

2. Results and discussion

2.1 Surface morphological studies of CdTe films

Fig. 1 (a-c) shows the SEM surface morphologies of CdTe films deposited at different various substrate temperatures. The images were measured by the SEM used on high multiples (20K). It can be found in Fig. 1 (a) that the CdTe film deposited at room temperature has a few worse crystalline grains (CdTe grains) with uniform size and clear grain boundary on the CdS substrates. Also, the CdTe grain is nanograin and the film surface has many structural defects. It is due to the role of the O_2 gas contains in the CdTe and CdS grain boundary thereby increasing the lattice mismatch between the CdTe layer and the CdS substrate [14].

It can be seen in Fig. 1 (b) that the size of the crystalline grains deposited at 200 ℃ is larger than that deposited at room temperature. The film deposited at 200 ℃ consists of circle shaped grains approximately 0.5μm in size and the grain desity is much denser. Also, many voids are reduced in the substrate heating process result in the decrease of the amount of shunting which limite the performance of the CdTe solar cell [15]. This heating treatment can remove the structural defects and nanograins in the CdTe film.

It can be seen in Fig. 1(c) that the large grains with well defined grain boundaries and some big cracks appear in the CdTe films at 400 ℃. Also, the grains show a hexahedronl structure and the film is rough. Meanwhile, the grain sizes changed from the 0.5 to 1.0 μm when the heated temperature increases from 200 to 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 from the difference of expansion coefficient of the film and substrate can lead to the aggregates of the cracks.

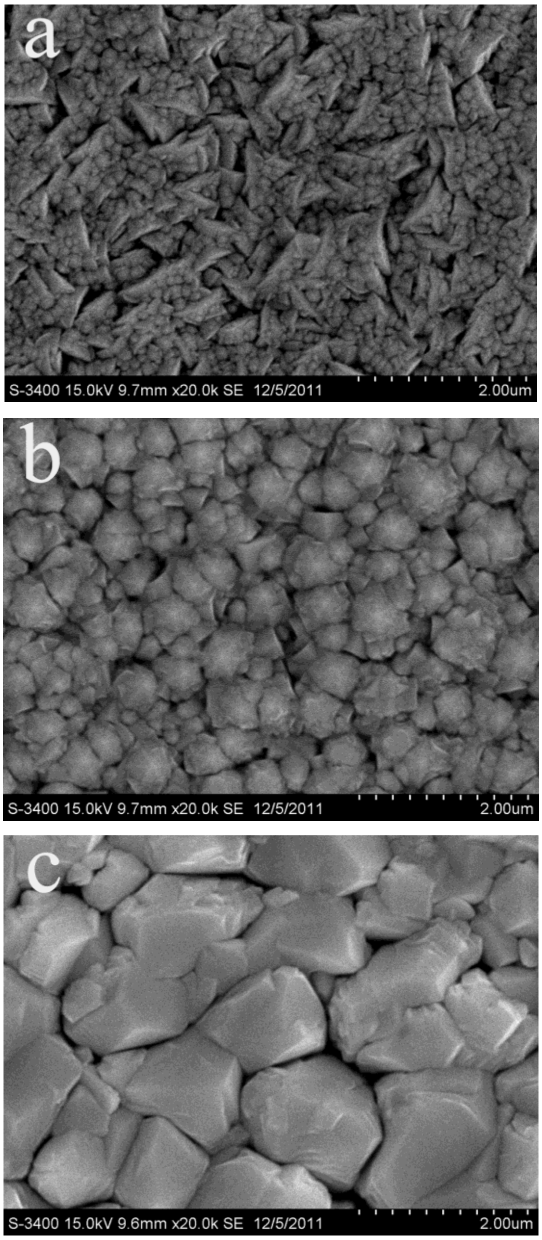

Fig. 1. SEM surface morphologies of CdTe films deposited at various substrate temperatures: (a) room temperature; (b) 200 ℃; (c) 400 ℃

2.2 Cross-section morphological studies of CdTe films

The cross-sectional morphologies of the CdTe films deposited at different substrate temperatures are shown in Fig. 2. It can be seen from Fig. 2(a), (b) that the CdTe film deposited at 200 °C has a much thicker section than the as-deposited film, which confirms the occurrence of regrowth and recrystallisation as indicated in the surface morphologies of CdTe films.

It can be also seen in Fig. 2(b) that the density of grains is increased with increasing grain sizes at the CdTe /CdS interface, which is considered to be because of the reconstruction and improvement in the CdTe crystals at the supplement of high energy for the heating process at 200 °C. For the films heated at 400 °C (Fig. 2(c)), it is seen that the interface is destroyed, with some cracks between the grains being present in the films, which implies that phase transformation occurs accompanied by evaporation of indium and selenium.

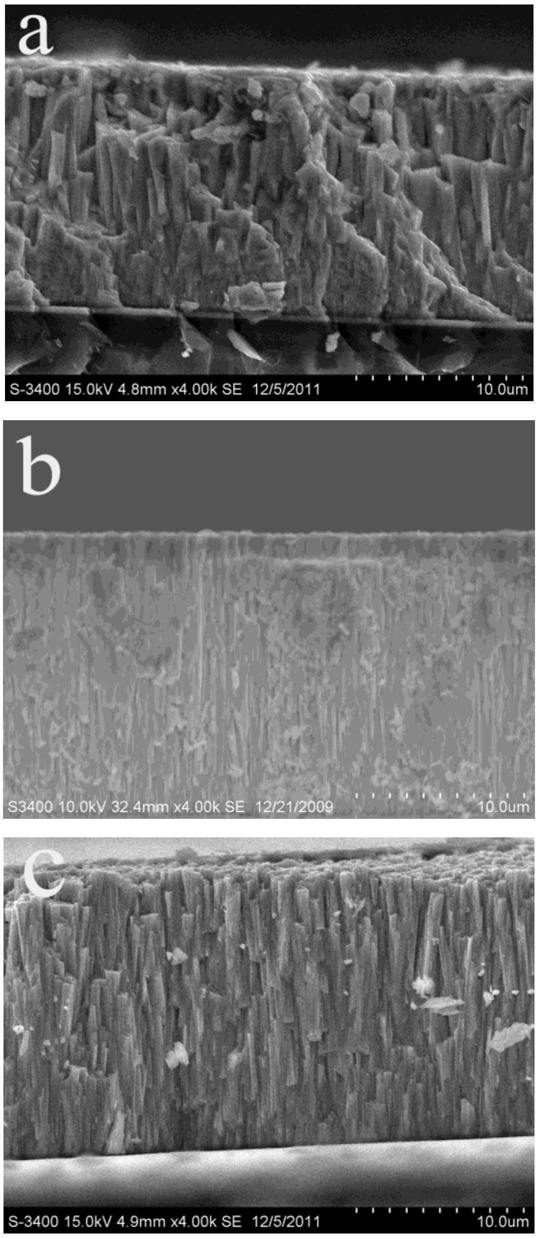

Fig. 2. SEM cross-section morphologies of CdTe films deposited at various substrate temperatures: (a) room temperature*; (b)* 200 ℃; (c) 400 ℃.

2.3 Optical absorption properties of CdTe films

Fig.3 shows the absorption spectra of CdTe films on different substrate temperatures in the wavelength range 200-1100 nm. It clearly shows an improvement in the optical performance f the CIS film after substrate heating process at 200 °C compared to that of the other heated temperatures. 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 absorption of the CdTe films at 200 ℃ exhibits good absorption to the sunlight not only in the in the visible region but also in the infrared region. However, at this optical absorption on the visible region range (600-800 nm) the film deposited at 200℃ is the best in all samples. According to this result, the improvement of cell performance at heating process of 200 ℃ may be mainly caused by the increase of the optical band gap during this heating process [16].

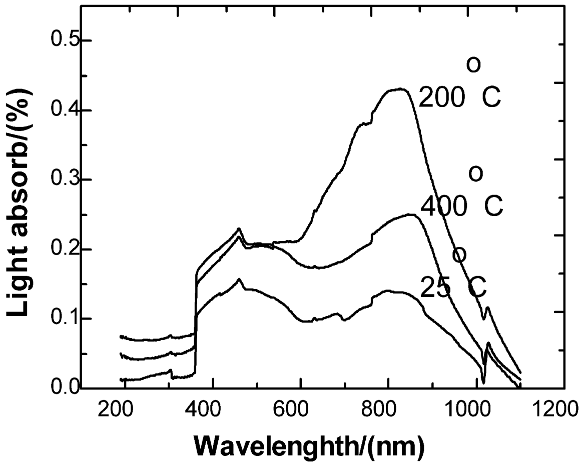

Fig. 3. Absorption spectra curves of CdTe films deposited at various substrate temperatures.

3. Conclusions

1) The surface morphologies results show that the increase of substrate temperature is in favor to change the grain size and structure shape. This heating treatment can remove the structural defects and nanograins in the CdTe film.

2) The section morphologies results implied the density of grains was increased with increasing grain sizes when substrate temperature increased from 25 to 200 ℃. This confirms the occurrence of regrowth and recrystallisation as indicated in the surface morphologies of CdTe films.

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 increase of the optical band gap is associated with the enhanced crystallinity of the CdTe films in the substrate heating treatment.

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*Corresponding author: jixin@sues.edu.cn