Properties of ZnTe Films Deposited with Different Substrate Temperature Using CSS Method

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Abstract. ZnTe films were prepared by close spaced-sublimation (CSS) method. The effects of substrate temperature on ZnTe films were investigated. The results showed cubic structure with strong (111) texture for all the films. Films with higher crystalline quality and larger grain size were obtained at higher substrate temperature. A red-shift of the optical bandgap and reduction of resistivity were observed with increasing substrate temperature.

1. Introduction
Zinc telluride (ZnTe), an important II-VI semiconductor, has recently received an increasing attention due to its excellent properties such as direct wide band-gap of 2.26 eV at room temperature, low electron affinity of 3.53 eV, high absorption coefficient of 105 cm⁻¹ and high electro-optic coefficient, which makes it a potential candidate for applications in optoelectronic devices and integrated optics such as solar cell, light emitting diodes, terahertz detectors [1-4].

To get Device-grade of ZnTe, a variety of film deposition techniques have to be applied [5], including thermal evaporation [6, 7], RF and DC sputtering [8], close spaced-sublimation (CSS) [9] and etc. Among those, CSS is a promising preparation technique for film deposition in terms of its rapid deposition rate and simple configuration. CSS method also offers many possibilities to adjust the preparation conditions to obtain uniform surface and large area thick films [10]. Up to now, relatively few results have been reported on preparation of ZnTe films using CSS method. The previous studies show that the substrate temperature for many deposition techniques is one of the key deposition parameters which has significant effects on the properties of ZnTe film [11].

In this paper, ZnTe films were deposited on glasses by CSS method. Substrate temperature dependent on properties of the ZnTe films were investigated systematically.

2. Experimental
ZnTe films were deposited on quartz glasses for 30 min with different substrate temperatures by CSS method. The sublimation source material was high-purity ZnTe powder (99.99%). The chamber was pumped down to the vacuum of 5×10⁻³ Pa before deposition. During the deposition, the source temperature was kept at 650 °C and the spacing between source and substrate was about 3 mm. The substrate temperature was varied from 200 °C to 500°C.

The crystallinity of the films was evaluated by X-ray diffraction (XRD, D/MAX-2200, Cu Kα, λ=0.15406 nm). The surface morphology was characterized by field-emission gun scanning electron microscopy (FESEM, Apollo 300) and the ZnTe composition was estimated using energy dispersive
spectrometer (EDS). Au electrode dots with a diameter of 2 mm were prepared by double ion beam sputtering, and current density-voltage (J-V) curves were measured using Keithley 2400 source meter. The absorption and transmission of the ZnTe films were measured by Jasco UV-570 spectrophotometer.

3. Results and Discussion

Figure 1 shows the XRD patterns of the ZnTe films. Compared with standard PDF card No. 15-0746, all ZnTe films exhibit a zinc blende structure with strong preferential (111) orientation. Most notably, the relative intensity of (111) peak increases apparently with increasing Ts. It suggests the better crystallinity and preferential orientation at higher Ts. Figure 2 shows a function of Ts with the position and full width at half maximum (FWHM) of the (111) peak. As shown in the Figure 2, the (111) peak positions are located at 2θ=25.019°, 25.280°, 25.259°, 25.221° for the films deposited at different substrate temperature, respectively. Compared with the case of Ts =200°C, the peak position of ZnTe (111) diffraction obviously shifts to large angle when Ts above 200 °C, which is very close to the standard value (2θ=25.259°) mentioned in JCPDS (15-0746). The figure also shows that the FWHM of (111) peaks decreases with increasing Ts, which implies the higher crystalline quality of the films at higher Ts.

![Figure 1. XRD patterns of the ZnTe films deposited at different substrate temperature (Ts). The inset is the enlargement of the (111) peak.](image1.png)

![Figure 2. A function of Ts with the position and FWHM of the (111) peak.](image2.png)

The variation in grain size and FWHM of the peak corresponding to the (111) plane as a function of $T_s$ is listed in Table 1. The grain size is calculated from the Scherrer relation [12]:

$$ D = \frac{0.89\lambda}{\beta\cos(\theta)} \tag{1} $$

where $D$ is the grain size of ZnTe films, $\beta$ is the FWHM of the (111) peak, $\lambda$ is the wavelength of

| $T_s$ [°C] | $2\theta$ [°] | FWHM [°] | Grain Size (D) [nm] |
|----------|--------------|----------|---------------------|
| 200      | 25.019       | 0.232    | 34.672              |
| 300      | 25.280       | 0.223    | 36.090              |
| 400      | 25.259       | 0.217    | 37.088              |
the X-rays (CuKα1 1.54056Å), and θ is the diffractive angle. From the Table 1, we can find that the grain size increases with increasing Ts, which indicates that the higher Ts can get the better crystallinity.

Figure 3 shows the SEM images of ZnTe films deposited at different Ts. From Figure 3, we can find that, with increasing Ts, the grain size increases, which is consistent with the XRD results.

![SEM images of ZnTe films deposited at different substrate temperature](image)

**Figure 3.** SEM images of the ZnTe films obtained at different substrate temperature.

It is well known that electrical properties of ZnTe films strongly depend on composition stoichiometry [13]. Table 2 presents the composition of ZnTe films obtained under different substrate temperatures estimated using energy dispersive spectrometer (EDS). We can find that at Ts =200 °C, the atomic ratio (Zn:Te=1.21) is greater than 1. However, above 200 °C, the ZnTe atomic ratio is close to 1. It is proposed that low substrate temperatures is a highly non-equilibrium conditions, which might produce defects in II-VI films [14]. The result indicates the improved crystalline quality of the ZnTe films at high Ts.

| Samples            | Ts [°C] | Atom rate [%] | Zn: Te |
|--------------------|---------|---------------|--------|
|                    |         | Zn            | Te     |        |
| Deposited-Sample   | 200     | 54.76         | 45.24  | 1.21   |
|                    | 300     | 48.79         | 51.21  | 0.95   |
|                    | 400     | 49.32         | 50.68  | 0.97   |
|                    | 500     | 49.16         | 50.84  | 0.97   |

The absorption spectra in the wavelength range of 450–700 nm for the ZnTe films obtained from different conditions are given in Figure 4. The fundamental absorption edges are clearly observed for
all samples. The absorption edge of the ZnTe films shifts to the longer wavelength with $T_s$ increasing from 200 °C to 500 °C.

The optical absorption at absorption edge corresponds to the electron transition from valence band to conduction band. The optical band-gap ($E_g$) of materials can be estimated from the change of the absorption coefficient ($\alpha$) in this edge region by using the function expressed as follows [15]:

$$\alpha h\nu = B(h\nu - E_g)^n$$  \hspace{1cm} (2)

where $h$ is Plank’s constant, $\nu$ is the frequency of the radiation, $B$ is a constant which depends on the nature of transition and $n$ is a number which can take the values 1/2, 3/2, 2 or more depending on whether the transition is direct-allowed, direct-forbidden, indirect-allowed or indirect-forbidden. By extrapolating the linear portion of the curves, we can get the optical band-gap, as shown in the Figure 5. It can be found that, with increasing $T_s$, the film optical band-gap decreases.

The I-V plots of the films deposited at different substrate temperatures was shown in Figure 6. A linear relationship can be observed indicating ohmic contacts between ZnTe films and Au electrodes. Compared the I-V curves of different samples, we can observe that the electrical resistivity of the films decreases with substrate temperature.

4. Summary
ZnTe films were deposited on to cleaned quartz glasses by CSS with different substrate temperature (200-500 °C). XRD results show that ZnTe films obtained have zinc-bende structure, and high $T_s$ are easier to obtain high-quality films. Films with higher crystalline quality and larger grain size were obtained at higher substrate temperature. All results indicate that increasing the substrate temperature can improve the quality of the ZnTe films effectively.

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Acknowledgements
This work was funded by Science and Technology Commission of Shanghai (No. 16010500500, 15520500200).