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Influence of substrate materials on the properties of CdTe thin films grown by hot-wall epitaxy

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Abstract

Growth of high-quality CdTe thin films by hot-wall epitaxy (HWE) under different temperature conditions and the control of their physical, electrical and structural properties have been examined by various ways. CdTe (1 1 0), $Zn_{0.04}Cd_{0.96}Te$ (1 1 1), $Hg_{0.2}Cd_{0.8}Te$ (1 1 1), Si (1 1 1) and BaF_2 (1 1 1) were used as substrates. The obtained films have the cut-off wavelength at 0.84–0.85 μm and the transmission of about 55–60% out of the fundamental absorption domain. The current–voltage investigations have shown that the contact properties strongly depend on the contact material and contact fabrication method and less depend on substrate materials. The film-specific resistances $(4–7)\times 10^4\,\Omega\,cm$ were determined. The CdTe deposition (layer thickness about 1000 Å) on $Cd_xHg_{1-x}Te$ resulted in significant increase in photodiodes electrical parameters. All samples showed the crystalline structure according to the XRD data with strong influence on lattice mismatch between CdTe and substrate materials. Atomic force microscope (AFM) investigations have shown a smooth and defect-free surface with a roughness range of 15–100 nm for 50 μm of basic length.

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Keywords: A1. Surface structure; A3. Hot wall epitaxy; A3. Thin film; B1. Cadmium telluride

1. Introduction

In this article, we report initial results for the growth of CdTe films on bulk CdTe, BaF_2, $Zn_xCd_{1-x}Te$, $Cd_xHg_{1-x}Te$ and Si substrates using hot-wall epitaxy (HWE). An important feature of this method is the growth conditions that can be

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close to the thermodynamic equilibrium [1]. Such conditions are provided by quasi-close growing area and by the appropriate choice of the three temperature parameters (T_{source}, T_{wall}, $T_{\text{substrate}}$). They help to keep the constant temperature gradient in the growing reactor [1,2].

In the last years significant attention has been given to the growth of CdTe thin films and to the control of their properties by different ways. CdTe has a wide range of applications from photovoltaic conversion, high-energy flux detectors, such as X-ray and γ-ray detectors, to electronic and optoelectronic devices [3]. Also, it is one of the most effective materials for producing solar cells with efficiency of about 16% and with 90% absorptivity of the incident light [4]. In addition, its close lattice match and chemical compatibility with $Cd_xHg_{1-x}Te$ ($0 \leqslant x \leqslant 1$) make CdTe an ideal substrate for growth of variable band gap IR detector material. On the other hand, CdTe thin films are one of the most suitable materials for passivation $Cd_xHg_{1-x}Te$-based detectors. In this application, CdTe films have advantages such as reliability during deposition onto the $Cd_xHg_{1-x}Te$ layers and constant zero-resistance area product values in different points of the array's surface [5,6]. The current lack of availability of high–-quality- and large-area CdTe substrates is generally considered as a major problem for different applications. This problem can be overcome by growing CdTe on an alternative substrate, which could then serve as a buffer layer for the subsequent synthesis [7].

Therefore, many investigations are carried out to improve the existing methods for manufacturing perfect CdTe thin films with reproducible thickness and morphology.

2. Experimental results and discussion

The CdTe thin films were deposited on several types of substrates: cleaved BaF_2 (1 1 1), polished Si (1 1 1), CdTe (1 1 0), $Zn_{0.04}Cd_{0.96}Te$. To investigate the properties of the fabricated films as a passivating material for IR technology, we carried out the CdTe film deposition on the $Cd_{0.2}Hg_{0.8}Te$ layers formed on $Zn_{0.04}Cd_{0.96}Te$ substrate by liquid-phase epitaxy (LPE). The choice of the substrate material was made after detailed consideration of the lattice parameters, chemical properties and surface morphology to obtain the films with different strain and defects structure and, as a consequence, with different physical properties. For heteroepitaxy, the lattice mismatch between the substrate and grown film is a serious problem which prevents the growth of high-quality films. The silicon substrates are used because of their transparency to IR radiation and their availability as large-area wafers with higher structural perfection. Before inserting into the growth reactor, the Si substrates were etched in HF solution for 1 min. Bulk CdTe and LPE $Cd_xHg_{1-x}Te$ layers were treated in HCl solution for 1 min as well. Then all substrates, except the $Cd_xHg_{1-x}Te$ layers, were preheated to a temperature of 393 K in the vacuum of 10^{-2} Torr for final substrate surface cleaning.

To obtain the films with the same morphology, but various thicknesses, different deposition time and same temperature parameters were used. The main goal of the investigation was to fabricate CdTe thin films with perfect crystal structure under a relatively low substrate temperature. The following temperature parameters were used: $T_{\text{source}} = 653\,\text{K}$; $T_{\text{wall}} = 673\,\text{K}$; $T_{\text{substrate}} = 323-393\,\text{K}$. The values of these parameters were chosen from the known data [7–15] and optimized experimentally. The deposition process was conducted in the high vacuum ($\sim 10^{-7}$ Torr). The deposition time was within 2–20 min. The overheating temperature of the substrate owing to deposition of materials vapor during the process was arranged about 2–30 K, depending on the deposition time (Fig. 1).

We used two methods to identify the film thickness: optical method (investigation of the transmission spectra interference in the 0.5–15 μm spectral range at 300 K) and mechanical (with the help of the electronic profilometer and metalomicroscope). These investigations identified that chosen temperature parameters have allowed to obtain the CdTe thin films with a growth rate of 0.03–0.05 μm/min.

Transmission spectra of CdTe thin films were investigated in the spectral range from 0.2 to

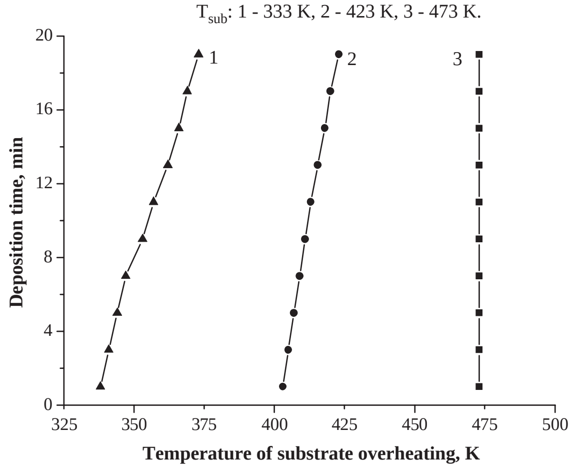

Fig. 1. Time–temperature dependences of the substrate overheating.

1.2 μm by Shimatsu UF-3100 device and from 1 to 10 μm by IKS-31 device. The cut-off wavelength of the CdTe films was obtained within 0.8–0.85 μm with transmission of about 55–60%. These results correspond to the known data for CdTe thin films prepared by other methods. The calculations showed that the band gap for the obtained CdTe thin films is equal to $E_g = 1.48$ eV, which is less than one for the bulk crystal, and can be related to the internal layer strains.

XRD measurements were carried out to make the conclusion of the structural properties (Fig. 2). CdTe films, which were prepared on the cleaved BaF_2 substrates had a polycrystal-like structure with (1 1 1), (2 1 1) and (5 1 1) orientations. Such structure can be explained by the damaged BaF_2 surface structure. It is known that cleaved BaF_2 surface is covered by steps and other defects. Thus, despite rather close lattice parameters (6.48 Å for CdTe and 6.2 Å for BaF_2), the CdTe thin films have polycrystalline-like structure. XRD data of CdTe films on Si substrate are shown in Fig. 2. In this case, the films have more perfect structure properties with two orientations: (1 1 1) and (5 1 1). Such difference between the samples prepared on Si and BaF_2 substrates can be explained by the surface perfection of the used Si substrate that allowed obtaining the high-quality CdTe films despite the large lattice mismatch (about 19%). Investigations of the crystalline structure of the CdTe films deposited on $Cd_xHg_{1-x}Te$ layers have shown that films have high-quality single crystalline structure with (1 1 1) orientation.

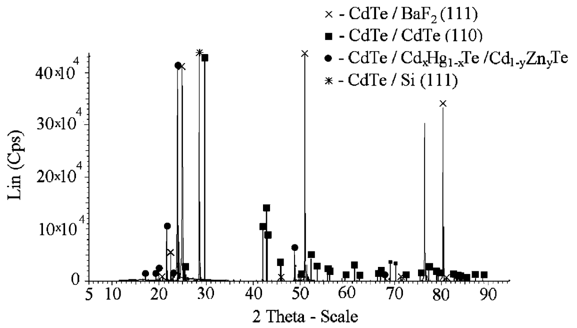

Fig. 2. XRD data of CdTe thin films deposited onto fresh cleaved BaF_2 (1 1 1), polished Si (1 1 1), $Cd_xHg_{1-x}Te$/$Zn_xCd_{1-x}Te$, bulk CdTe (1 1 0).

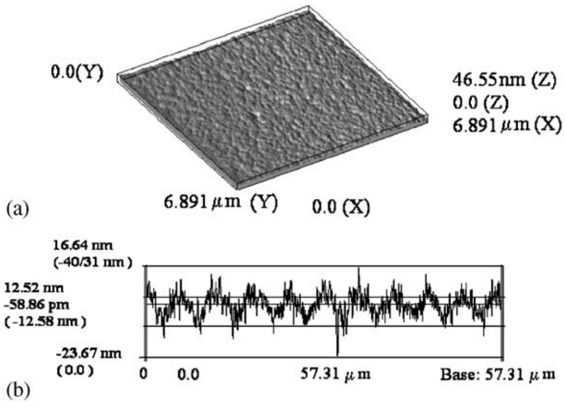

Fig. 3. AFM image (a) and profile of surface points distribution on heights (b) of the CdTe thin film deposited on BaF_2 substrates.

Also, structural properties of CdTe thin films deposited on different substrates were investigated by the atomic force microscope (AFM) technique. Fig. 3 demonstrates the 3D AFM image (a) and linear profile of surface points distribution on heights (b) of CdTe, which has been grown on BaF_2 (1 1 1) substrate. Significant lattice mismatch results in relief formation with uniform distribution of surface imperfections (~12 nm). Some structural parameters, viz., root-mean-square roughness (R_q), mean roughness (R_a), mean roughness of the profile by 10 points (R_z), maximum roughness height (R_{max}), were calculated for

Table 1
Surface roughness of the CdTe films deposited on different substrates

Samples	R_q (nm)	R_a (nm)	R_z (nm)	R_{max} (nm)
CdTe/BaF$_2$	5.041	4.001	30.38	40.31
CdTe/Si	15.55	8.422	99.65	129.8
CdTe/Zn$_x$Cd$_{1-x}$Te	8.317	5.830	16.17	51.98

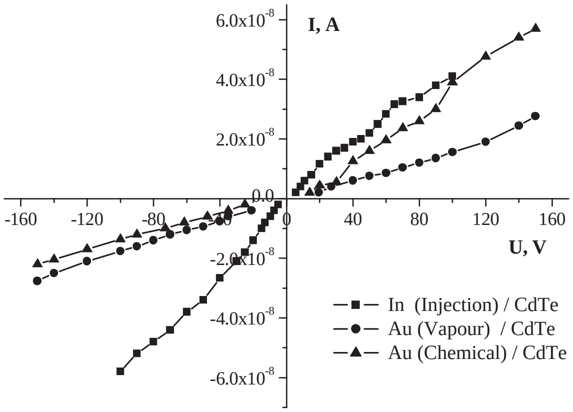

Fig. 4. CdTe films current–voltage characteristics at 300 K.

CdTe/BaF$_2$, CdTe/Si, CdTe/Zn$_{0.04}$Cd$_{0.96}$Te films from surface profile (Table 1). As seen, the parameter R_z has increased with raising in the lattice mismatch values.

Current–voltage characteristics were carried out to investigate the electrical contact properties of the CdTe films. Au and In were used as a contact metal. The contacts were created by the following methods: vacuum deposition of evaporated metals and chemical deposition from the solution. It was determined that the *I–V* characteristics of the prepared samples depended on the contact material and contact fabrication method. It was shown (Fig. 4) that In contacts prepared by chemical deposition formed Schottky barrier-like characteristics. Au contacts were prepared by both methods: chemical and vacuum deposition. The properties of Au contacts were determined to be strongly dependent on the contact preparation method. Au contacts formed by the chemical deposition from the solution create a Schottky barrier. On the other hand, Au contacts deposited onto CdTe films in vacuum display the ohmic properties. Apart from the current–voltage characteristics the specific resistance was measured. These measurements showed that the specific resistance was within $(4–7)\times10^4\,\Omega\,$cm, depended on the contact material and its preparation method.

Surface passivation of Cd$_{0.2}$Hg$_{0.8}$Te layer ($d\sim20\,\mu$m) was investigated by means of the CdTe thin film ($d\sim1000\,\text{Å}$). As a result, substantial improvements of photodiodes electro-physical parameters were found.

3. Conclusion

The CdTe thin films were prepared by HWE on substrates: CdTe (1 1 0), Zn$_{0.04}$Cd$_{0.96}$Te (1 1 1), Hg$_{0.2}$Cd$_{0.8}$Te (1 1 1), Si (1 1 1) and BaF$_2$ (1 1 1). The films were grown with the next temperature parameters: $T_{source} = 653\,$K; $T_{wall} = 673\,$K; $T_{substrate} = 323-393\,$K. Obtained films had the cut-off wavelength at 0.84–0.85 μm and transmission of about 55–60% out of the fundamental absorption domain. All samples showed a well-pronounced crystalline structure according to the XRD measurements. The microstructure and roughness of the thin films surface was analyzed by AFM. The *I–V* investigations showed that the contact properties strongly depended on the contact material and contact fabrication method. The obtained samples had the specific resistance $(4–7)\times10^4\,\Omega\,$cm. The CdTe passivation layers have been obtained for IR photodiodes based on LPE Cd$_{0.2}$Hg$_{0.8}$Te.

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