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Effect of deposition temperature on structural, morphological and optical properties of ZnTe thin films

I. Lungu[1,*], V. V. Zalamai[2], E. I. Monaico[2], L. Ghimpu[3], and T. Potlog[1]

[1] Physics and Engineering Department, Moldova State University, Chisinau, Republic of Moldova
[2] National Center for Materials Study and Testing, Technical University of Moldova, Chisinau, Republic of Moldova
[3] Institute of Electronic Engineering and Nanotechnologies, Academy of Sciences of Moldova, Chisinau, Republic of Moldova

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ABSTRACT

This paper describes technological processes developed for less studied ZnTe thin films prepared by close space sublimation method, without an additional transport agent gas, for controlling their structural and optical properties. The enhanced oxygen incorporation depends on the source–substrate growth conditions. ZnTe thin films fabricated in the source-substrate temperature interval mentioned here crystallize in a cubic zincblende structure preferentially oriented along the [111] reflection plane. As the source temperature increases, the energy dispersive X-ray spectroscopy shows that the tellurium content increases, while the oxygen decreases. The values of the optical band gaps vary in interval from 2.21 eV up to 2.22 eV with variation of the source temperature, while variation of the substrate temperature leads to the band gap value decrease from 2.24 to 2.14 eV. The photoluminescence spectra of the ZnTe:O thin films are dominated by the red emission bands localized at 1.73 eV and 1.82 eV. This study will serve as a basis for future efforts to develop intermediate-band solar cells with improved conversion efficiency.

Introduction

Zinc telluride (ZnTe) is a chalcogenide of A_2B_6 binary compounds with value of the direct bandgap of 2.26 eV at 300 K [1, 2]. ZnTe crystallizes in zincblende structure (F43m space group) and has *p*-type conductivity. Particularly, ZnTe is an interesting material, widely used in light-emitting diodes [3, 4], laser screens [5] and thin films transistors [6–8]. At the same time, ZnTe is a promising material for green/UV light detection due its superior sensitivity to Si and GaAs [9–11]. Furthermore, doping with oxygen, chromium, ZnTe can possess intermediate band (IB) structure [12], which makes it a promising material for photovoltaic devices due to a theoretical efficiency of 63% [13]. Luque and Marti found the maximum efficiency of 63.2%, for a bandgap of 1.95 eV with the

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Address correspondence to E-mail: ionlungu.usm@gmail.com

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IB 0.71 eV from either the valence or conduction band [14].

ZnTe thin films are fabricated by different physical deposition methods (substrate temperature $\geq$ 500 °C), such as molecular beam epitaxy (MBE) [15], vapor transport deposition (VTD) [16], as well as low-temperature deposition methods (substrate temperature $\leq$ 450 °C), such as glancing angle deposition (GLAD) [17], magnetron sputtering [2], electrodeposition (ED) [18], high vacuum evaporation (HVE) [19], close-spaced sublimation (CSS) method [20] and electron beam evaporation (EBE) [21]. Among the main advantages of the CSS method over other vacuum technologies are homogeneous growing, relatively low evaporation temperature, high deposition rate (up to 10 μm/min), synthesis of thin films with superior quality and low-cost industrial scalability [22, 23].

Farooq et al. [24] performed a comparative study on the structural and optical properties of ZnTe doped with Ag by CSS and (EBE) techniques. Comparison of structural properties shows better crystal orientation and highly dense films with very small porosity, small crystallite size using EBE than CSS technique, while morphological analysis demonstrated highly uniform particle size distribution with less porosity for CSS verses EBE, with highly rough surfaces after Ag doping. The authors of the publication [25] revealed that stoichiometric composition and good crystallinity can be achieved in CSS fabricated ZnTe films by increasing the substrate temperature (T_{sub}), which are basic requirements for device quality films. Park et al. [27] reported low resistive *p*-type ZnTe films, obtained by CSS using Na_2Te as a sodium source for doping, resulting in film resistivity less than 1 Ω cm with hole concentration of 6×10^{17} cm^3. The hole mobility increases with Na_2Te content due to an increase in grain size of ZnTe. Moreover, ZnTe proved to be low resistive, stable, and efficient back contact for polycrystalline ZnTe/CdTe/CdS/ITO solar cells [26]. The reported values of 4.28 eV electron affinity and 5.78 eV work function of *p*-type CdTe thin films, form Schottky barrier with metals [27]. However, an ohmic contact is highly desirable and represents the key issue in the fabrication of CdTe based photovoltaic cells [28]. Therefore, ZnTe is the best candidate to fulfill these requirements and compatibility with the CdTe based tandem solar cells [29]. The authors of Refs. [30, 31] synthesized undoped and Cu-doped ZnTe thin films, at optimized parameters by sublimation through the CSS technique using additionally an ion exchange process. The reproducible polycrystalline cubic structure of the Cu-doped ZnTe thin films with preferred orientation (111) was obtained. The resistivity of thin films changed from $\sim 10^7$ Ω cm for undoped ZnTe to $\sim$ 1 Ω cm for Cu-doped ZnTe thin film. The calculated concentration increased by two orders of magnitude, up to $1.4 \times 10^{11}/cm^2$ for Cu-doped ZnTe thin films in comparison with undoped ZnTe thin film of $\sim 4 \times 10^9/cm^2$. These results predicted that Cu-doped ZnTe thin film can be used as an ideal, efficient, and stable intermediate layer between metallic and absorber back contact for the CdTe heterojunction thin film solar cell technology. This affirmation is demonstrated by the authors of the following publications [32, 33]. So, it has been demonstrated that ZnTe can be deposited using the CSS technique, which is the most common method to deposit CdTe in both, research and photovoltaic industry.

In this paper, the main objective consists in systematic study of the physicochemical features and structural properties in function of substrate–source temperatures and impurity–defect interaction in the wide bandgap ZnTe polycrystalline thin films obtained by CSS method. The second task is to establish the relationship of these processes and to identify the right way to control the composition, structure with necessary set of optoelectronic material properties. Understanding these features are important due to the observed phenomena and processes in polycrystalline thin films that should play an important role in future development of IB solar cells. Based on reported results in this paper, following the intermediate band model, a strategy that will allow designing IB solar cells with optimal photovoltaic efficiency values will be developed.

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