



Growth and characterization of $\text{Zn}_{1-x}\text{Cd}_x\text{Te}_{1-y}\text{O}_y$ highly mismatched alloys for intermediate band solar cells



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ABSTRACT

Quaternary $\text{Zn}_{1-x}\text{Cd}_x\text{Te}_{1-y}\text{O}_y$ (ZnCdTeO) alloys with Cd and O contents of $x < \sim 0.7$ and $y < \sim 0.03$, respectively, were grown on ZnTe substrates by molecular beam epitaxy. Structural x-ray diffraction measurements indicate that the degree of the lattice distortion strongly depends on the alloy composition. Lattice relaxation is observed in the 400 nm-thick ZnCdTeO layer with a lattice mismatch of more than 1.5%. The optical absorption of ZnCdTeO strongly depends on the alloy composition and the spectral dependence of the absorption coefficient is well described by the electronic band structure resulting from anticrossing interaction between localized O level and the conduction band of $\text{Zn}_{1-x}\text{Cd}_x\text{Te}$ matrix. Measurements of the photovoltaic performance of two intermediate band solar cell structures indicate an importance of the conduction band alignment and the location of the intermediate band relative to the upper conduction band.

1. Introduction

Dilute oxide $\text{ZnTe}_{1-x}\text{O}_x$ (ZnTeO) is one of the highly mismatched alloys (HMAs) which is a class of materials whose electronic band structures are dramatically modified through the substitution of a relatively small fraction of host atoms with an element of very much different electronegativity or size [1–6]. In ZnTeO, the incorporation of a small amount of isoelectronic O leads to the formation of a lower intermediate (E_-) and an upper conduction (E_+) subbands as a result of an anticrossing interaction between localized states of O and the conduction band (CB) of ZnTe matrix as described by the band anticrossing (BAC) model [1]. The energies of the three possible photon absorption edges between the valence, E_- , and E_+ bands of ZnTeO fit quite well into a large portion of the solar spectrum providing a material envisioned for the multi-band, single junction, high efficiency photovoltaic devices [7–11]. The band gap combination can be further optimized to better match the solar spectrum by incorporating Cd into ZnTeO, leading to the decrease of the energy gaps [12–15].

In $\text{Zn}_{1-x}\text{Cd}_x\text{Te}_{1-y}\text{O}_y$ (ZnCdTeO), both the energy positions and the nature of E_- and E_+ bands strongly depend on Cd and O contents because the conduction band minimum (CBM) of ZnCdTe shifts downward with increasing Cd content whereas O level (E_0) stays unchanged,

relative to the vacuum level [13–15]. The energy gaps between valence band and E_- and E_+ bands decrease with increasing Cd content and the nature of both E_- and E_+ bands changes largely at around Cd content $x \sim 0.3$ where the CBM of ZnCdTe moves below E_0 [15]. In order to utilize ZnCdTeO for intermediate band solar cells (IBSCs), it is important to understand how structural and optical properties of ZnCdTeO depend on Cd and O contents, especially at the Cd content around $x \sim 0.3$.

Recently, we have reported the growth of ZnCdTeO layers with a wide range of Cd content with Cd mole fraction between 0 and 0.7 by molecular beam epitaxy (MBE) [15]. In these experiments [15], only the Cd flux was changed during the growth while the O radical supply condition was kept constant. As a result, the Cd content in the ZnCdTeO layers was found to increase almost linearly with increasing the Cd flux ratio whereas O content decreases gradually with increasing Cd content, indicating that the incorporation ratio of O into ZnCdTe lattice decreases with increasing Cd content. The optical transition energies of the layers determined from photorefectance spectra were consistent with those calculated based on the BAC model. The optical absorption properties of some layers were also investigated. However, a systematic study on the compositional dependence of structural and optical properties were not carried out due to a lack of control on the

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composition of Cd and O independently in different samples [15]. More importantly, no attempt has been made on fabricating a prototype IBSC structure to investigate photovoltaic (PV) properties using a ZnCdTeO layer.

Here, we report the MBE growth and characterization of ZnCdTeO layers with Cd and O contents of $x=0-0.7$ and $y=0-0.03$ in order to clarify the compositional dependence of the properties of ZnCdTeO layers. In addition, preliminary PV results of IBSCs fabricated using ZnCdTeO layers are reported.

2. Experimental

ZnCdTeO layers were grown on ZnTe(001) and α -Al₂O₃(0001) substrates by a conventional MBE system with a radio frequency radical cell for O. The background pressure of the growth chamber is less than 6×10^{-8} Pa. 7N Zn, 6N Cd and 6N Te were used as source materials. Both ZnTe(001) and α -Al₂O₃(0001) substrates were ultrasonically cleaned in organic solvents prior to wet-etching using a Br-methanol solution for ZnTe(001) and a H₂SO₄:H₃PO₄ (3:1) solution for α -Al₂O₃(0001). A low-temperature ZnTe buffer layer was grown at 250 °C for 5 min, followed by a growth of ZnCdTeO layer at 400 °C. The Cd flux ratio f ($= [\text{Cd}]/([\text{Zn}] + [\text{Cd}])$) was changed between 0 and 0.8 to control Cd composition of ZnCdTeO layer. The flux ratio of Te to Zn and Cd ($= [\text{Te}]/([\text{Zn}] + [\text{Cd}])$) was set to 1 or 2. The O radical supply conditions were also changed by changing the RF power between 90 and 110 W whereas O₂ flow rate was kept constant at 0.2 sccm. The growth time was 60 min and the typical film thickness was 400 nm.

Cd content x was determined from energy dispersive x-ray spectroscopy (EDX) measurements. $\omega-2\theta$ scans of symmetrical 004 and asymmetrical 224 reflections were recorded using a high-resolution x-ray diffraction (XRD) system to determine the in-plane and out-of-plane lattice constants, a_{\parallel} and a_{\perp} . Then, O content y was estimated by assuming Vegard's law using a relaxed lattice constant a_{ZnCdTeO} calculated from a_{\parallel} and a_{\perp} and Cd content x determined by EDX, as reported previously [12].

Secondary ion mass spectroscopy (SIMS) was performed to obtain depth profiles of the layer using Cs⁺ as a primary ion. The absorption coefficient α was derived from optical transmittance and reflectance spectra measured using a double-beam spectrophotometer in the wavelength range of 300–2000 nm. In order to avoid the influence from ZnTe substrates, ZnCdTeO layers on α -Al₂O₃(0001) substrates were used for EDX and optical measurements.

3. Results and discussion

3.1. Compositional and structural properties

Fig. 1(a) shows the variation of Cd content in ZnCdTeO layers grown under $[\text{Te}]/([\text{Zn}] + [\text{Cd}])$ flux ratio of 1 and 2 as a function of the Cd flux ratio. It is seen that the Cd content in the ZnCdTeO layers increases almost linearly with increasing Cd flux ratio. The Cd content is higher for films grown under the higher flux ratio $[\text{Te}]/([\text{Zn}] + [\text{Cd}]) = 2$. This implies that Cd is more easily incorporated under Te-rich conditions. Similar tendencies were reported in the MBE growth of ZnCdSe where the mole fraction of Cd in ZnCdSe increased with increasing Se flux [16].

In order to confirm the compositional uniformity, the atomic depth profile of ZnCdTeO layer with $x=0.31$ and $y=0.005$ was measured by SIMS. The results are shown in Fig. 1(b) and (c), and the yield ratios of O/Te and Cd/Zn are also shown in the insets of Fig. 1(b) and (c), respectively. It is confirmed that the Zn, Cd, Te, and O are uniformly distributed throughout the layer. The O peak observed at a depth of 0.42 μm originates from the residual native oxide existing at the interface between ZnTe buffer layer and p -ZnTe substrate. Even though we removed the native oxide by a thermal cleaning procedure and confirmed the oxide removal by the change of the RHEED pattern from halo-like to spot pattern before the growth of buffer layer, the SIMS result still indicated the presence of residual native oxide at the interface. However, after the growth of a 40 nm-thick buffer layer, RHEED pattern changed to a streak-like pattern. This suggests that the residual native oxide does not significantly affect the crystallinity. Nevertheless, we expect that the crystalline quality of the over layer may be improved further by a more efficient removal of the native oxide before the buffer growth. This will be investigated further.

Fig. 2(a) and (b) show the variation of XRD profiles at around the (004) diffraction peak with Cd content for ZnCdTeO layers with high ($y \sim 0.02$) and low ($y \sim 0.006$) O contents, respectively, on ZnTe(001) substrates. In both cases, the diffraction peak from ZnCdTeO (004) plane shifts to lower angle with increasing Cd content, indicating an increasing lattice parameter associated with replacement of Zn by larger Cd atoms [15]. In ZnCdTeO layers with low O contents shown in Fig. 2(b), the similar peak shift from ZnCdTeO (004) plane was observed although 2 diffraction peaks appear in the XRD patterns of ZnCdTeO with $x \geq 0.3$. Also, a very weak second peak is observed on the lower angle side of the ZnCdTeO (004) diffraction peak in ZnCdTeO

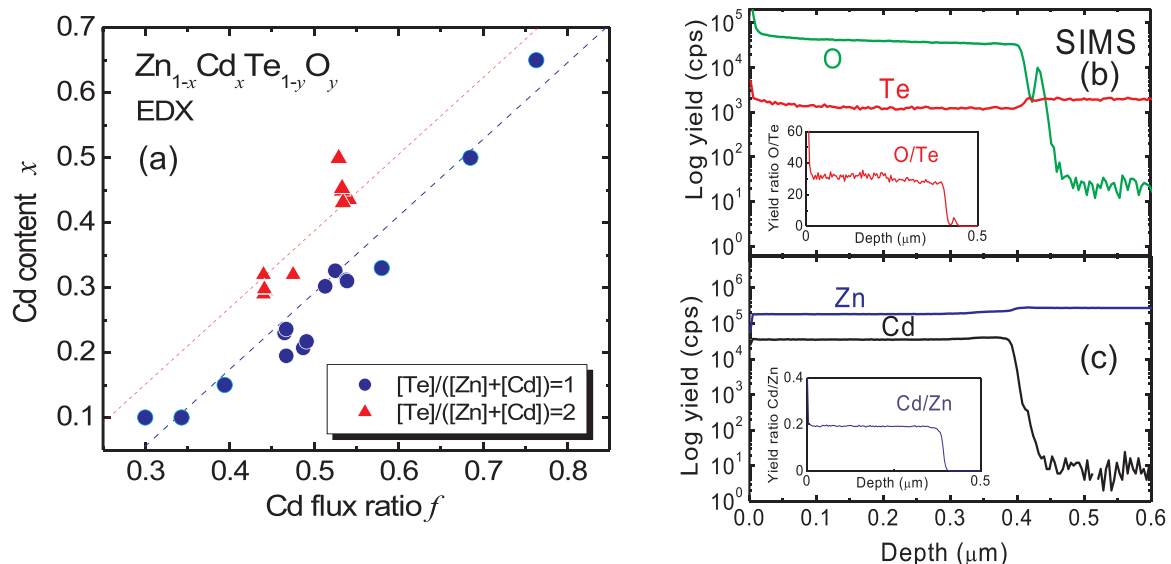


Fig. 1. (a) Variation of Cd content in ZnCdTeO layers grown under $[\text{Te}]/([\text{Zn}] + [\text{Cd}])$ flux ratio of 1 and 2 as a function of the Cd flux ratio. SIMS depth profile of (b) O and Te (c) Zn and Cd for ZnCdTeO layer with $x=0.31$ and $y=0.005$. The inset in (b) and (c) show the yield ratios of O/Te and Cd/Zn, respectively.

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