Phys. Status Solidi C **12**, No. 9–11, 1211–1214 (2015) / **DOI** 10.1002/pssc.201510068

physica status solidi c
www.pss-c.com
current topics in solid state physics

Growth and characterization of CdTe absorbers on GaAs by MBE for high concentration PV solar cells

Ozan Arı*[,1], Mustafa Polat[1], Merve Karakaya[2], and Yusuf Selamet[1]

[1] Department of Physics, Izmir Institute of Technology, Izmir 35430, Turkey
[2] Department of Material Science and Engineering, Izmir Institute of Technology, Izmir 35430, Turkey

Received 20 May 2015, revised 2 October 2015, accepted 5 October 2015
Published online 21 October 2015

Keywords CdTe, single crystal, solar cell, MBE growth

* Corresponding author: e-mail ozanari@gmail.com, Phone: +90 232 750 7676

CdTe based II-VI absorbers are promising candidates for high concentration PV solar cells with an ideal band gap for AM1.5 solar radiation. In this study, we propose single crystal CdTe absorbers grown on GaAs substrates with a molecular beam epitaxy (MBE) which is a clean deposition technology. We show that high quality CdTe absorber layers can be grown with full width half maximum of X-ray diffraction rocking curves (XRD RC) as low as 227 arc-seconds with 0.5 % thickness uniformity that a 2 µm layer is capable of absorbing 99 % of AM1.5 solar radiation. Bandgap of the CdTe absorber is found as 1.483 eV from spetroscopic ellipsometry (SE) measurements. Also, high absorption coefficient is calculated from the results, which is ~5 x 10^5 cm^{-1} in solar radiation spectrum.

© 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

1 Introduction High concentration photovoltaic (PV) solar cell systems are important in such a way that they combine less material usage with high solar conversion efficiency. III-V multi-layer structures are most widely used absorbers for high concentration PV solar cells [1]. However, structural defects such as point defects and dislocations in III-V multi-layers severely limit solar cell efficiencies which are usually attributed to the dominant covalent bond characteristic between Ga and As atoms [1]. For II-VI semiconductor absorbers materials, on the other hand, optical properties are expected to be less affected from the dislocations and other structural defects which is believed to be related with higher ionic character of bonding between the II and VI atoms than that of III-V atoms [2]. CdTe based II-VI absorbers are promising candidates for high concentration PV solar cell systems. The efficiency of the polycrystalline CdTe solar cell is reached 21.5 % [1] while theoretical limit is ~ 32% [2]. Low solar cell efficiencies of the polycrystalline CdTe based solar cells are correlated with the low open circuit voltages (V_{oc}). This problem is thought to be related with structural defects in the polycrystalline CdTe absorbers and interfaces [3]. In the early 1990s, there was a brief interest in CdTe single crystal solar cell devices [3]. However, solar cell community lost interest in CdTe single crystal solar cells due to high production costs and small area of the suitable substrates. In the late 2000s, a new approach to form single and multi-junction single crystal CdTe solar cell devices is reported [3].

Dislocations are the structural defects in the CdTe absorber and hence act as trap centers for the free electrons [4]. These trap zones acts like recombination centers for the electrons and holes which they greatly reduce the solar cell efficiency. In this study we propose an environment friendly method for single crystal CdTe(211) absorber deposition on GaAs(211)B substrates by employing a high purity CdTe source in an MBE system. Surface structure and growth mode were monitored and analyzed *in situ* by reflection high energy electron diffraction (RHEED) system. In order to evaluate crystal quality high resolution X-ray diffraction (XRD) rocking curve (RC) measurements were performed around surface symmetric (422) reflections from [0-11] azimuth. Electronic properties of the CdTe absorber were obtained with SE technique. Thickness uniformity of the CdTe absorbers

© 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

over the wafer were evaluated from the interference fringes at the transmission spectra in near infrared (NIR) region.

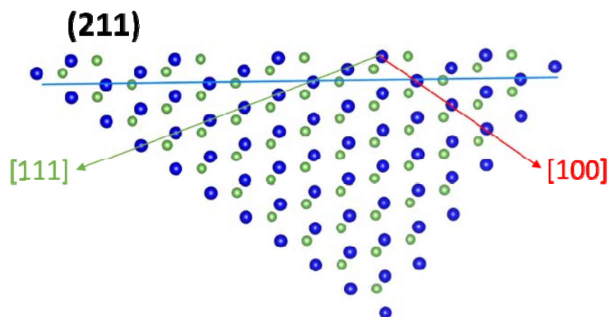

Figure 1 Ball model of the (211) surface of the GaAs.

2 MBE growth We grew CdTe thin absorber layers on 2 x 2 cm^2 GaAs(211)B epiready substrates by MBE with 99.99999% (7N) purity CdTe material. Lattice mismatch between the CdTe and GaAs is 14.6 %. High index (211) surface contains (111) and (100) crystal planes as they form step edges at the surface. Step edge geometry of the (211) surface has advantage of having uniform energetically favorable nucleation sites [5,6] (Fig. 1). (211) surface orientation plays an important role to suppress twining and other structural defects during the growth of the CdTe absorbers [7]. Ideal epitaxial (211) layers grow on GaAs(211)B substrates with ~3° tilting towards [-111] azimuth which allows a better lattice parameter match between the (4-2-2) planes of the CdTe and GaAs [8]. The (4-2-2) plane is perpendicular to the (111) orientation and interplanar distance of (4-2-2) is proportional to the bond distance in (111) orientation. In this context, a better lattice match in (4-2-2) orientation leads to a better match of the (111) planes of GaAs and CdTe [9]. Also, surface termination (As or Ga) of the substrate in the polar (211) surface may affect the surface morphology and chemical structure of the protective oxide layer of the epiready wafers.

Protective oxide layer of GaAs epiready wafers were thermally removed under As overpressure at 585 ^{o}C surface temperature which were measured by pyrometer. The sample was then cooled to the growth temperatures as the temperature was monitored with a non-contact thermocouple at the back side of the sample. Growth was performed in three steps; initially a nucleation layer was deposited at 365 ^{o}C which was followed by anneal at 525 ^{o}C for 5 minutes. Finally, the growth of the absorber layer was initiated at 460 ^{o}C with a 4.1 x 10^{-10} Torr background pressure.

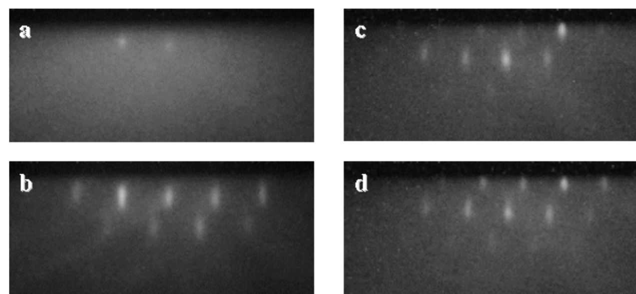

Figure 2 *In situ* RHEED patterns from [0-11] direction during the growth process; (a) before, and (b) after deoxidation of the GaAs(211)B surface, (c) CdTe initiation layer growth, (d) CdTe absorber layer growth.

3 Results Deoxidation, nucleation, annealing and absorber layer growth of surface was *in situ* monitored with RHEED. Evolution of the RHEED patterns during deoxidation were observed from [0-11] azimuth with a CMOS detector based system and diffraction spot intensities were recorded. RHEED pattern from the protective oxide layer of the GaAs substrate is shown in Fig. 2a, which indicates an amorphous oxide structure. After the thermal deoxidation of the GaAs substrate, RHEED pattern exhibit long streaks which points that surface is atomically smooth and ready for growth (Fig. 2b). In Fig. 2c and d, nucleation layer and absorber CdTe layer RHEED patterns are given, respectively. It is seen from the figures that rough growth of the nucleation layer turns into smoother surface with annealing. The growth of the CdTe absorber layer at this surface exhibits RHEED pattern of a highly crystalline and atomically smooth surface.

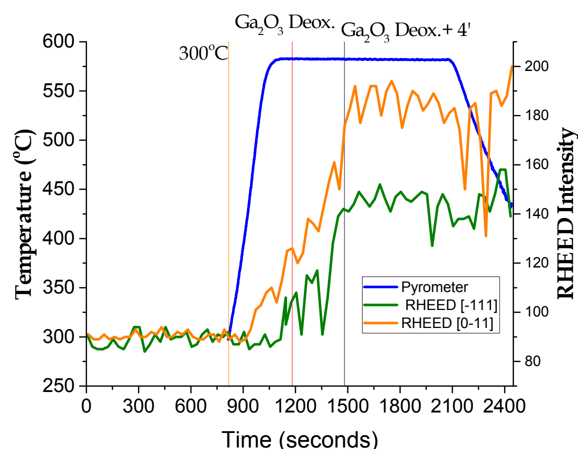

Figure 3 *In situ* RHEED pattern spot intensity evolution with respect to surface temperature and temperature from [0-11] and [-111] azimuths.

Recorded RHEED spot intensities during deoxidation of the GaAs surface is shown in Fig. 3. RHEED spot intensities were recorded from two different surface azimuths [0-11] and [-111]. RHEED spot intensity changes were observed during the surface temperature change from

© 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

300 °C to 585 °C. After that point, RHEED pattern has shown no pattern and intensity changes. First RHEED spot intensity increase is related with the As_2O_3, As_2O_5 and Ga_2O desorption from the surface while the second one is related to more tightly bonded Ga_2O_3 desorption from the GaAs surface [10].

Crystal quality of the CdTe absorber layer is determined by employing XRD technique. High resolution four-crystal XRD RC measurements are performed around the CdTe (422) surface reflection from [0-11] azimuth. A measurement result is shown in Fig. 4. RC peak is modelled with a PearsonVII curve fit which has adjusted R^2 value of 0.9994. Full width half maximum (FWHM) of the RC is 227.4 ± 0.5 arc-seconds. Threading dislocation density of the CdTe absorber is calculated from the FWHM of the CdTe (422) reflection as 1.28×10^8 cm^{-2} [11].

Thickness uniformity of the CdTe absorber layer is determined from the transmission map which was obtained with Fourier transform infrared (FTIR) spectroscopy system. Thickness is calculated by evaluation of the interference fringes in near infra-red region (10500-650 cm^{-1}) of the transmission spectra which were taken at 7 × 7 points in an approximately 11.5 × 11.5 mm^2 zone of the CdTe absorber layer. Evaluated thickness map from the CdTe absorber layer is shown in Fig. 5. The deviation in the CdTe absorber layer thickness was ±0.005 μm with 2.335 μm average layer thickness.

The optical properties of the CdTe absorber layer were measured with SE technique. Dielectric functions of the CdTe absorber layer is simulated with a multi-oscillator model. Thickness of the layer was calculated as 2.2940 ± 0.0004 μm which is in good agreement with the thickness obtained from the FTIR measurements. Calculated refractive index and extinction coefficient of the CdTe absorber layer is shown in Fig. 6. Sharp increase in the extinction coefficient around the ~1.5 eV is remarkable and it is related to the photon absorption of the material. Additionally, absorption coefficient is calculated from the extinction coefficient in order to determine the band gap of the CdTe absorber layer and light absorbing properties of the CdTe layer (Fig. 7). Absorption coefficient of the CdTe layer is found as ~5×10^5 cm^{-1} in NIR and UV-VIS region. Also, the calculated bandgap of the CdTe absorber layer is found to be 1.483 eV at room temperature. Both absorption coefficient and bandgap of the CdTe absorber layer are indicators of the highly quality single crystal absorber layer [4].

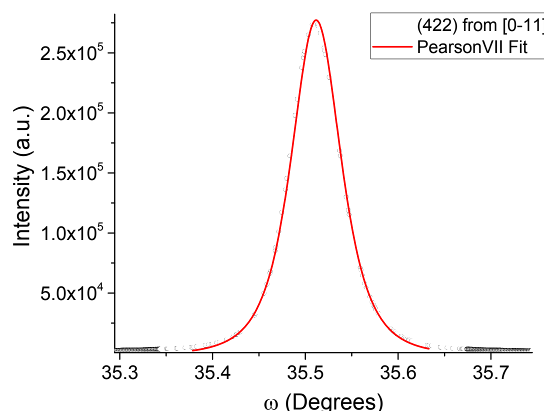

Figure 4 Four crystal high resolution XRD RC measurement around the CdTe (422) symmetric reflection from [0-11] azimuth.

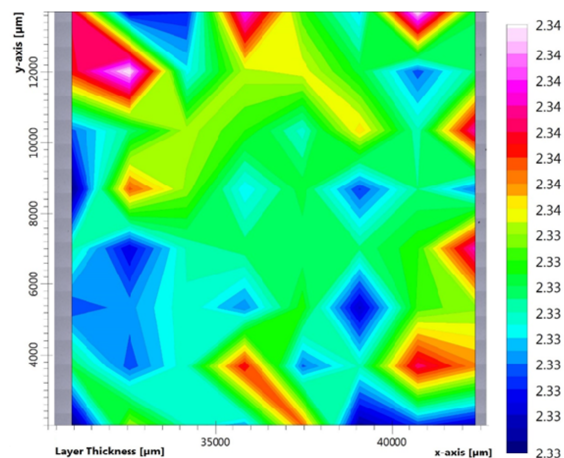

Figure 5 Thickness map of the CdTe absorber layer of approximately 11.5 × 11.5 mm^2 area.

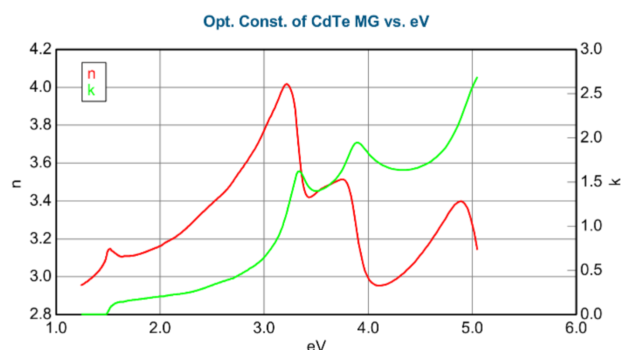

Figure 6 Refractive index (n) and extinction coefficient (k) of the CdTe absorber layer.

© 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

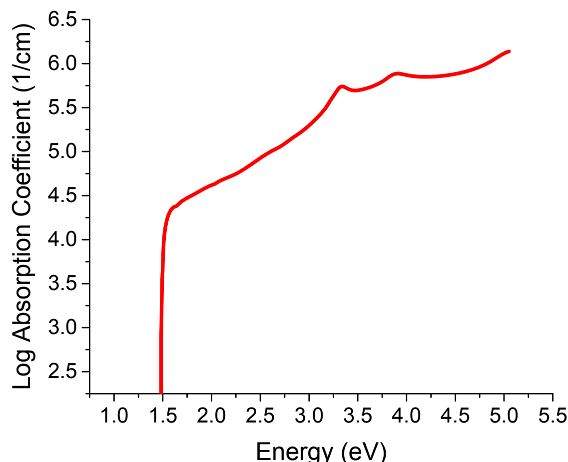

Figure 7 Absorption coefficient of the CdTe absorber layer as function of photon energy.

4 Conclusions In this study, we show that highly crystalline CdTe absorber layer can be grown on GaAs substrates with XRD RC FWHM 227 arc-seconds and 1.28×10^8 cm^{-2} dislocation densities at about 2.3 µm thickness. Low dislocation density value suggests very low trap centers in CdTe absorber layer hence possible high solar cell efficiencies with this layer. Also thickness uniformity of the CdTe absorber layer is found as 0.5% for 2.335 µm layer. On the other hand, absorption coefficient for this layer is calculated as $\sim 5 \times 10^5$ cm^{-1} for solar radiation spectrum which is in good agreement with bulk value [4]. In addition, bandgap of the CdTe layer is found as 1.483 eV. Therefore, MBE-grown single crystal CdTe absorbers have great potential for high concentration PV solar cell devices with low dislocation densities grown by a clean production method.

Acknowledgements We are grateful to Orhan Öztürk from Izmir Institute of Technology for XRD measurements.

References

[1] National Renewable Energy Laboratory (NREL), Effic. Chart (2015).
[2] W. Shockley and H.J. Queisser, J. Appl. Phys. **32**, 510 (1961).
[3] J.W. Garland, T. Biegala, M. Carmody, C. Gilmore, and S. Sivananthan, J. Appl. Phys. **109**, 102425 (2011).
[4] A. Luque and S. Hegedus, Handbook of Photovoltaic Science (John Wiley & Sons Ltd., 2003).
[5] N.K. Dhar, P.R. Boyd, M. Martinka, J.H. Dinan, L. a. Almeida, and N. Goldsman, J. Electron. Mater. **29**, 748 (2000).
[6] G. Brill, Y. Chen, N.K. Dhar, and R. Singh, J. Electron. Mater. **32**, 717 (2003).
[7] X.J. Wang, S. Tari, R. Sporken, and S. Sivananthan, Appl. Surf. Sci. **257**, 3346 (2011).
[8] S.Y. Woo, G.A. Devenyi, and R.N. Kleiman, Appl. Phys. Lett. **132103**, 1 (2013).
[9] Y. Nakamura, N. Otsuka, M.D. Lange, R. Sporken, and J.P. Faurie, Appl. Phys. Lett. **60**, 1372 (1992).
[10] D. Allwood, S. Cox, N. Mason, R. Palmer, R. Young, and P. Walker, Thin Solid Films **412**, 76 (2002).
[11] S. Fahey, Selective Area Epitaxy of CdTe on Nanopatterned Substrates, University of Illinois at Chicago, 2012.

© 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim