Correlative characterization of dislocation defects and defect clusters in GaAs and CdTe solar cells by spatially resolved optical techniques and high-resolution TEM

Q. Chen,[1] B.S. McKeon,[2] J. Becker,[2] S. Zhang,[1] C.-K. Hu,[1,3] T.H. Gfroerer,[4] M.W. Wanlass,[5] Y.-H. Zhang,[2] D.J. Smith,[2] and Y. Zhang [1,+]

[1]University of North Carolina at Charlotte, Charlotte, NC 28223, USA
[2]Arizona State University, Tempe, Arizona 85287, USA
[3]Wuhan University of Technology, Wuhan, Hubei 430070, China
[4]Davidson College, Davidson, NC 28035, USA
[5]National Renewable Energy Laboratory, Golden, CO 80401, USA

[+]Author for correspondence: yong.zhang@uncc.edu

Abstract — **An array of correlative and spatially-resolved techniques, including electroluminescence, photoluminescence, Raman, I-V curve, and high-resolution TEM, have been performed on both GaAs and CdTe solar cells, to study the impact of individual dislocation defects and defect clusters on device performance, the dependence of the impact on the device operation conditions, and the microscopic structures of the defects. This approach offers quantitative and definitive correlation between the atomistic structure of a defect and its effects in a real device.**

I. INTRODUCTION

The ultimate constraint for a solar cell or practically any semiconductor device to reach its theoretical efficiency limit is the quality of the active material, namely the inevitable presence of structural defects. It is common knowledge that defects will degrade the device performance. However, in a real device, because of the challenges in carrying out *operando* characterization at an individual defect level, it is generally unclear how an individual defect will affect the device performance, how the impact depends on the device operation conditions, how the impact varies from one defect to another, and how the variation in impact is correlated to the microscopic scale defect structure. Recently, we have made a concerted effort to correlate PL imaging/chemical etching/SEM imaging in a CdTe epilayer, which revealed that etch pits did not always match the dark spots visible in PL imaging [1]. Although the results of the PL imaging were somewhat better at reflecting the impact of defects in a real device, the PL process still did not reveal how the carriers were generated, injected, or extracted in real electronic or optoelectronic devices, such as transistors, photo-detectors, solar cells, and LEDs. This background of prior work motivated us to carry out more comprehensive characterization, from optical, electrical, to structural, all at the individual defect level.

In this work, we have addressed the above questions through investigating and characterizing the impact of individual dislocations in GaAs and CdTe solar cells by applying an array of correlative and spatially-resolved techniques, including electroluminescence (EL), photoluminescence (PL), Raman, and current-voltage (I-V) characteristics [2]. Furthermore, we have determined the atomic-scale defect structures using high-resolution TEM for the same defects that were first characterized with these techniques.

II. EXPERIMENTAL DETAILS

A GaAs solar cell that consists of many independent sub-cells was used in this study. The cell structure contains, from the top to the bottom, a 80 nm *n*-type GaAs contact layer, 50 nm n-type GaInP window layer, 40 nm n-type GaAs emitter layer, 3 μm p-type GaAs absorber layer, 50 nm *p*-type GaInP back-surface confinement layer, 80 nm *p*-GaAs buffer layer, then *p*-type GaAs substrate. Two contact electrodes, made out of Au, are deposited onto the topmost and bottom most layer. The GaAs epilayers grown under similar conditions were found to have very low dislocation-type defect densities on the order of 10^2 cm^{-2} or 1 mm^{-2} [3]. A CdTe device with comparable dislocation density is also studied [4]. Here we use the GaAs device to illustrate our approach.

In the past, a low magnification PL imaging system was typically used to first identify the approximate location of an individual defect in the GaAs layer of the bare GaAs/GaInP double heterostructure, then high-resolution PL mapping was used to determine its accurate position, followed by detailed optical studies [3, 5]. However, the GaAs active or absorber layer in the fabricated device yielded a much weaker PL signal, which made it difficult to find any significant defect in this device using the PL imaging technique. EL imaging is instead used in this study, since it is found to offer much higher

978-1-5386-8529-7/18/$31.00 ©2018 IEEE

sensitivity and efficiency in locating isolated defects that are actually detrimental to the photo-generated and electrically injected carriers. Once a likely defect, typically shown as a dark spot on the EL image, is identified, Raman and PL mapping are carried out near the EL dark spot to confirm that the identified feature is indeed a real structural defect of the absorber layer, as opposed to some other irregularity (e.g., processing induced blemishes on the device surface), because the defect of interest has unique spectroscopy features. By analyzing the measured light I-V curves obtained by separately focusing a 532-nm laser beam at the defect site and away, we are able to assess directly the impact of a single defect on the key solar cell performance parameters, including short circuit current I_{sc}, open circuit voltage V_{oc}, fill factor FF, shunt resistance R_{sh}, and energy conversion efficiency η.

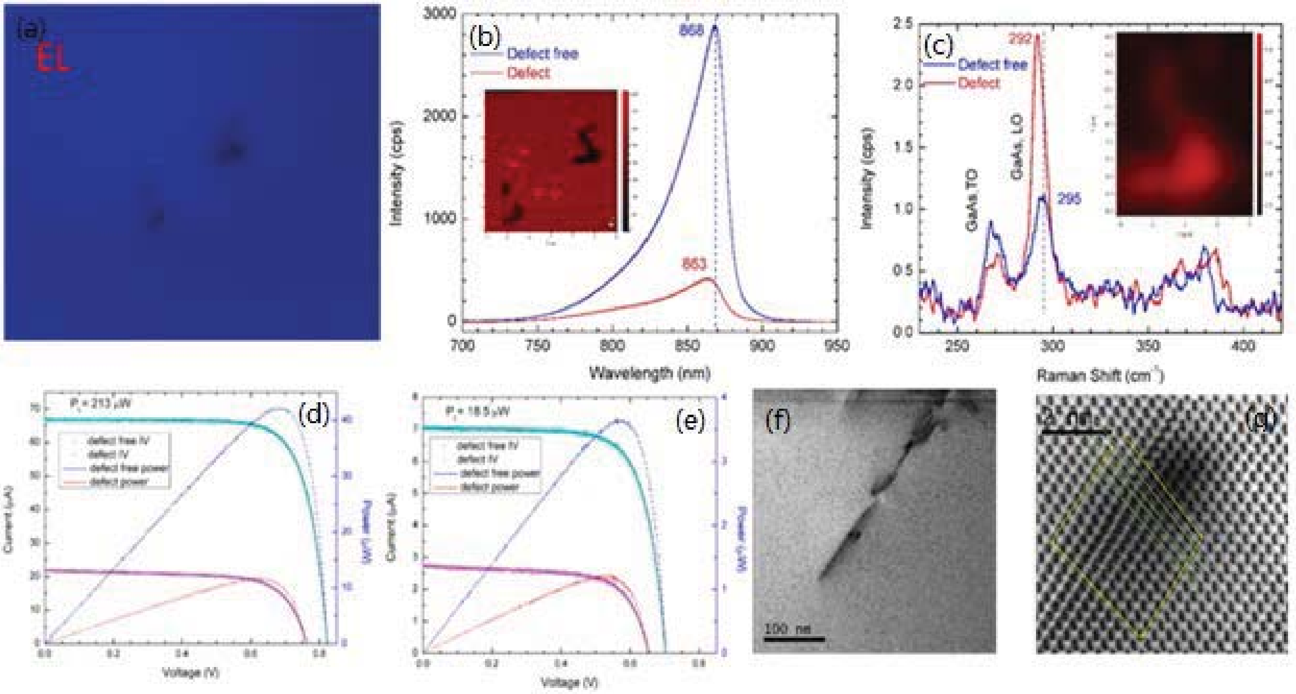

Figure 1. Set of EL, PL, Raman spectra, I-V curves, and TEM images and obtained from dislocation defect present at GaAs solar cell surface.

III. RESULTS AND DISCUSSION

Figure 1 is a set of EL, PL, Raman spectra, I-V curves, and TEM images obtained from an individual defect. The dark regions in the EL image reveal the positions and shape of the possible defects. The PL mapping, the inset of Fig. 1(b), shows better intensity contrast between the defects and general areas. As expected, the PL intensity from a defect spot is much lower than that of the defect-free spot. Surprisingly, the PL peak energy at 868 nm blue shifts to 863 nm at the defect spot. Usually, one would expect a lower peak energy at the defect when there are fewer carriers to fill up the electronic states. Fig. 1(c) compares their Raman spectra. The defect-free spot shows two standard GaAs Raman modes: 295 cm^{-1} for longitudinal optical (LO) mode and 270 cm^{-1} for transverse optical (TO) mode, whereas the defect Raman reveals a sharper, stronger and red-shifted LO mode at 292 cm^{-1} and a slightly weaker TO mode. These findings are rather surprising, because intuitively one would expect the defect exhibiting local structure distortions, to yield broader and weaker spectroscopy features. We have concluded that the shift in the LO frequency is due to the difference in the carrier density between the defect and defect-free site, manifested through LO phonon-plasmon coupling [6]. The details about the Raman analysis will be presented elsewhere [C.-K. Hu et al., to be published]. From the I-V curves shown in Figs. 1 (d) and (e), we find that a single defect can drastically degrade the light-to-electricity conversion efficiency when light is illuminated right at the defect site compared to when it is illuminated at a defect-free site, through reducing key solar cell parameters, such as short circuit current (I_{sc}), open circuit voltage (V_{oc}), fill factor (FF), and shunt resistance (R_{sh}), to different degrees. The impact is found to depend on the illumination intensity as well the specific defect. For example, the I_{sc} is found to be reduced by ~68% from the defect-free site to the defect site with an illumination laser power of 213 μW, and the efficiency drops by ~72.1%. At 18.5 μW, the changes are ~ 61% in I_{sc} and ~66.5% in efficiency.

This study provides insights for both the fundamental understanding of defect physics and the practical knowledge of the adverse effects of the defects at the single defect level.

ACKNOWLEDGEMENT

The work at UNCC was supported by ARO/MURI (W911NF-10-1-0524) and ARO/Electronics (W911NF-16-1-0263). YZ acknowledge the support of Bissell Distinguished Professorship at UNCC.

REFERENCES

[1] H. Liu, Y. Zhang, Y. Chen, and P. S. Wijewarnasuriya, Confocal Micro-PL Mapping of Defects in CdTe Epilayers Grown on Si (211) Substrates with Different Annealing Cycles. *Journal of Elec Materi* **43**, 2854 (2014).

[2] Q. Chen, and Y. Zhang, The reversal of the laser-beam-induced-current contrast with varying illumination density in a Cu2ZnSnSe4 thin-film solar cell. *Applied Physics Letters* **103**, 242104 (2013).

[3] T. H. Gfroerer, Y. Zhang, and M. W. Wanlass, An extended defect as a sensor for free carrier diffusion in a semiconductor. *Applied Physics Letters* **102**, 012114 (2013).

[4] Y. Zhao, M. Boccard, S. Liu, J. Becker, X.-H. Zhao, C. M. Campbell, E. Suarez, M. B. Lassise, Z. Holman, and Y.-H. Zhang, Monocrystalline CdTe solar cells with open-circuit voltage over 1 V and efficiency of 17%. *Nature Energy* **1**, 16067 (2016).

[5] F. Chen, Y. Zhang, T. H. Gfroerer, A. N. Finger, and M. W. Wanlass, Spatial resolution versus data acquisition efficiency in mapping an inhomogeneous system with species diffusion. *Sci. Rep.* **5**, 10542 (2015).

[6] A. Mooradian, and G. B. Wright, Observation of the Interaction of Plasmons with Longitudinal Optical Phonons in GaAs. *Physical Review Letters* **16**, 999 (1966).