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RPPR Final Report
as of 04-May-2021

Agency Code: 21XD

Proposal Number: 69053EL **Agreement Number: W911NF-16-1-0263**

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Title: Correlative study of defects in semiconductors (Research Topic Area: 4.3 Electronic Sensing)
Begin Performance Period: 02-May-2016 **End Performance Period:** 30-Nov-2020
Report Term: 0-Other

Submitted By: Ph.D. Yong Zhang Email: Yong.Zhang@uncc.edu
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STEM Degrees: **STEM Participants:**

Major Goals: (1) to achieve a comprehensive understanding of specific types of structural defect (e.g., threading dislocations) in terms of their microscopic structure and impact on electronic and optical properties; (2) to understand how a collection of defects can affect the mesoscale (or macroscale) electrical and optical behavior of optoelectronic materials; and (3) to explore the potential impact of defects on device performance in different applications and under different operating conditions.

Accomplishments: see uploaded pdf file.

Training Opportunities: At least five ph.D students had worked on this project and supported partially by this project.

Results Dissemination: One paper has been published during this period:
Qiong Chen, Brandon S. McKeon, Sunny Y. Zhang, Fan Zhang, Changkui Hu, Timothy H. Gfroerer, Mark W. Wanlass, David J. Smith, and Yong Zhang, Impact of individual structural defects in GaAs solar cells: a correlative and in operando investigation of signatures, structures, and effects, Adv. Opt. Mat. 9, 2001487 (2020).

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: PD/PI
Participant: Yong Zhang
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
National Academy Member: N

RPPR Final Report
as of 04-May-2021

Participant Type: Co PD/PI
Participant: David J. Smith
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
National Academy Member: N

Participant Type: Co PD/PI
Participant: Yong-Hang Zhang
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
National Academy Member: N

ARTICLES:

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
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Volume: 185 Issue: 5 First Page #: 200
Date Submitted: 8/29/17 12:00AM Date Published: 1/18/17 9:48PM
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Article Title: Kinetic energydependenceofcarrierdiffusioninaGaAsepilayer studied bywavelengthselectivePLimaging
Authors: S. Zhang, L. Q. Su, J.Kon, T. Gfroerer, M. W. Wanlass,Y.Zhang
Keywords: Photoluminescence imaging, Electron diffusion, Thermal distribution, Diffusion length, GaAs thin film
Abstract: Photoluminescence (PL) imaging has been shown to be an efficient technique for investigating carrier diffusion in semiconductors. In the past, the measurement was typically carried out by measuring at one wavelength (e.g., at the band gap) or simply the whole emission band. At room temperature in a semiconductor like GaAs, the band-to-band PL emission may occur in a spectral range over 200 meV, vastly exceeding the average thermal energy of about 26 meV. To investigate the potential dependence of the carrier diffusion on the carrier kinetic energy, we performed wavelength selective PL imaging on a GaAs double hetero-structure in a spectral range from about 70 meV above to 50 meV below the bandgap, extracting the carrier diffusion lengths at different PL wavelengths by fitting the imaging data to a theoretical model. The results clearly show that the locally generated carriers of different kinetic energies mostly diffuse together, maintaining the same thermal distribution throughout ...
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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
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Volume: 7 Issue: 1 First Page #:
Date Submitted: 8/30/18 12:00AM Date Published: 6/1/18 8:00AM
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Article Title: Overcoming diffusion-related limitations in semiconductor defect imaging with phonon-plasmon-coupled mode Raman scattering
Authors: Changkui Hu, Qiong Chen, Fengxiang Chen, T. H. Gfroerer, M. W. Wanlass, Yong Zhang
Keywords: Phonon, Plasomn, Raman, Photoluminescence, defects, resolution
Abstract: Carrier diffusion is of paramount importance in many semiconductor devices, such as solar cells, photodetectors, and power electronics. Structural defects prevent such devices from reaching their full performance potential. Although alarge carrier diffusion length indicates high material quality, it also implies increased carrier depletion by an individual extended defect (for instance, a dislocation) and obscures the spatial resolution of neighboring defects using optical techniques. For commonly utilized photoluminescence (PL) imaging, the spatial resolution is dictated by the diffusion length rather than by the laser spot size, no matter the spot is at or below the diffraction limit. Here, we show how Raman imaging of the LO phonon-plasmon-coupled mode can be used to recover the intrinsic spatial resolution of the optical system, and we demonstrate the effectiveness of the technique by imaging defects in GaAs with diffraction-limited optics, achieving a 10-fold improvement resolutio
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Date Submitted: 9/28/18 12:00AM Date Published: 9/1/18 12:00AM
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Article Title: Micro-Raman Three-Dimensional Thermometry with Diffraction-Limit Spatial Resolution for
Authors: T. Park, Yong-Jing Guan, Zhi-Qiang Liu, Yong Zhang
Keywords: 3D Raman thermometry, LED, defect, in-operando
Abstract: Confocal micro-Raman microscopy performed in the transparent spectral region of a semiconductor can, in principle, be used for operando three-dimensional (3D) thermometry with optical diffraction-limit spatial resolution. However, when applied to high-power GaN-based light-emitting diodes (LEDs), the applicability is hindered by the often strong secondary electroluminescence in the visible spectral region that overwhelms the Raman signal. We develop a “split-time-window” scheme that can mimic the continuous wave operation but without the interference of the secondary emission, which allows us to carry out noninvasive 3D temperature profiling and comprehensive thermal analyses of the whole device at any operation current. The technique is applied to an (InxGa1?x)N/GaN LED to extract its 3D temperature distribution when operated at 350 mA with ?m-scale resolution when using a 532-nm laser. We show that although a conventional technique can yield a reliable average temperature difference
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Volume: 185 Issue: First Page #: 200
Date Submitted: 9/28/18 12:00AM Date Published: 5/1/17 12:00AM
Publication Location:
Article Title: Kinetic energy dependence of carrier diffusion in a GaAs epilayer studied by wavelength selective PL imaging
Authors: S. Zhang, L.Q. Su, J. Kon, T. Gfroerer, M.W. Wanlass, Y. Zhang
Keywords: Photoluminescence imaging, Electron diffusion, Thermal distribution, Diffusion length, GaAs thin film
Abstract: Photoluminescence (PL) imaging has been shown to be an efficient technique for investigating carrier diffusion in semiconductors. In the past, the measurement was typically carried out by measuring at one wavelength (e.g., at the band gap) or simply the whole emission band. At room temperature in a semiconductor like GaAs, the band-to-band PL emission may occur in a spectral range over 200 meV, vastly exceeding the average thermal energy of about 26 meV. To investigate the potential dependence of the carrier diffusion on the carrier kinetic energy, we performed wavelength selective PL imaging on a GaAs double hetero-structure in a spectral range from about 70 meV above to 50 meV below the bandgap, extracting the carrier diffusion lengths at different PL wavelengths by fitting the imaging data to a theoretical model. The results clearly show that the locally generated carriers of different kinetic energies mostly diffuse together, maintaining the same thermal distribution throughout the
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Partners

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I certify that the information in the report is complete and accurate:
Signature: Yong Zhang
Signature Date: 4/26/21 10:01PM

Final Report (05/2/2016 - 11/30/2020)

Title: Correlative study of defects in semiconductors

PI: Yong Zhang (UNC-Charlotte)

Co-PIs: David J. Smith and Yong-Hang Zhang (ASU)

April 26, 2021

The primary goal of this project was to address a few questions that all defect studies were supposed to answer but it was rarely possible to do so in the multiple-decade-long defect research.

The questions are:

(1) How would an individual defect affect device performance? People had been able to "see" individual defects, including their atomistic structures, but typically the defects were not studied in a functioning device.

(2) How does the impact of the defect in a device varies from one defect to another? One can speculate that one type of defect might be worse than the other, but it is impractical to construct specific defects with known microscopic structures in a device then compare their impacts.

(3) How does the impact depend on the device operating conditions? For instance, one type of defect might be more problematic at low carrier density, whereas the other might be more detrimental at high carrier density, which may correspond to the situations of a solar cell operating at one sun vs. 1,000 suns or a LED operating at 10 mA vs. 1,000 mA.

A traditional approach to defect studies, which we refer to as a ***parallel*** mode, is to cut a grown wafer into multiple pieces for different investigations, as illustrated by **Fig. 1**. A major limitation of this approach is that *either* the defect investigated by structural characterization techniques was not the same defect that was affecting the device performance (i.e., they were presumed to be similar defects but nevertheless from different pieces of the materials) *or else* the defect was not characterized under operating conditions.

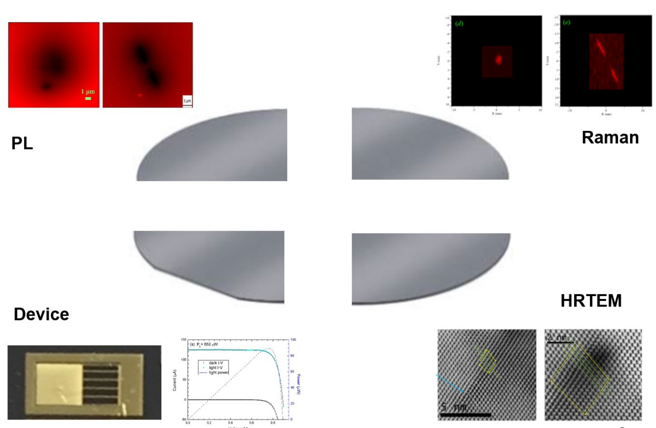

Fig. 1 A parallel mode of defect study.

In this study, we have taken a totally different and novel approach, referred to as a ***series*** mode, as illustrated by **Fig. 2**, namely after the material growth, firstly to fabricate a device, then identify defect(s) on the device, measure the effects on device performance under different operating conditions using multiple correlative spatially resolved spectroscopy techniques, and finally mark the defect(s) for structural characterization using atomically-resolved TEM techniques. The novelty of our work primarily lies in using a "series" approach as opposed to the usual "parallel" approach. Additionally, the success of this much more challenging approach requires an ability to seamlessly integrate multiple characterization techniques. As far as we know, this is the first such attempt.

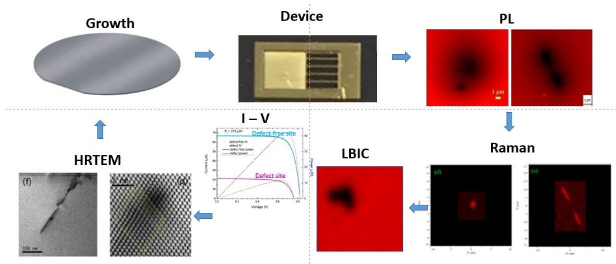

Fig. 2 A series mode of defect study.

This work has allowed us, for the first time after many decades of defect study, to address and answer those questions mentioned above. Two technologically important material systems GaAs and CdTe were selected as prototype systems for illustrating the ability to achieve unprecedented insights that would not be obtainable using the conventional material characterization approaches. A comprehensive paper entitled "*Impact of individual structural defects in GaAs solar cells: a correlative and in operando investigation of signatures, structures, and effects*" has been published in Advanced Optical Materials.[1] This paper confirms that we have accomplished the original, primary goal of this project.

We believe this work will encourage many more similar efforts to address practical device performance issues for many types of device applications, ranging from solar cells, photo-detectors, light emitting devices, to power electronic devices.

Additionally, we have contributed to the understanding and characterization of defects in semiconductor materials and devices through the publications of a few important papers that are briefly described below:

(i) The first comprehensive comparative study on the optoelectronic properties between three prominent PV materials: GaAs, CdTe, and organic-inorganic hybrid perovskite, including their PL efficiencies and carrier diffusion lengths in multiple orders in magnitude of illumination density. The work has been published in Materials Today.[2]

(ii) New insight to the over three-decade controversy regarding whether or not the electron-phonon coupling (EPC) is weakened or not in semiconductor nanostructures. Our thorough investigation on the bulk, thin-film, and nanowire ZnTe samples has revealed that much of the conflicting results in the literature were likely extrinsic in nature related to defects, and the EPC can be controlled and tuned by defects incorporated either during the growth or after growth by laser illumination. This work has been published Physical Review Applied as a Letter.[3]

(iii) It is often difficult to know the carrier density (e.g., electron density n) in a material, because it cannot be directly measured. Instead, one can measure the emission rate or injection rate that is related to dn/dt. For the first time, we performed Raman imaging near individual dislocation defects in GaAs epilayers and solar cells, and were able to obtain the electron density distribution near the defects by analyzing the LO-phonon-plasmon (LPP) coupled mode; and by combining the information from Raman and PL imaging data to further extract the hole density distributions near the defects. A paper was published in Light: Science & Applications.[4]

(iv) A number of techniques are available to measure device temperature, from perhaps the most straightforward method – IR imaging to more sophisticated methods, such as lock-in thermography, thermo-reflectance, and Raman thermometry. These techniques are typically only capable of probing surface temperature of a device. We have developed an *in-operando* micro-Raman 3D thermometry with diffraction-limit spatial resolution that can probe, for instance, how the epilayer/substrate interfacial imperfection in a LED may lead to local heating, potentially device failure. The paper has been published in Physical Review Applied.[5]

We hope that these novel approaches or techniques can find broader applications in material research and real-world device characterization. Some can be further developed to better match diverse device operation conditions.

References

[1] Q. Chen, B. S. McKeon, S. Y. Zhang, F. Zhang, C. Hu, T. H. Gfroerer, M. W. Wanlass, D. J. Smith, and Y. Zhang, Impact of Individual Structural Defects in GaAs Solar Cells: A Correlative and In Operando Investigation of Signatures, Structures, and Effects. *Advanced Optical Materials* **9**, 2001487 (2021).

[2] F. Zhang, J. F. Castaneda, S. Chen, W. Wu, M. J. DiNezza, M. Lassise, W. Nie, A. Mohite, Y. Liu, S. Liu, D. Friedman, H. Liu, Q. Chen, Y.-H. Zhang, J. Huang, and Y. Zhang, Comparative studies of optoelectrical properties of prominent PV materials: Halide perovskite, CdTe, and GaAs. *Materials Today* **36**, 18 (2020).

[3] Y. Yi, J. K. Marmon, Y. Chen, F. Zhang, T. Sheng, P. S. Wijewarnasuriya, H. Zhang, and Y. Zhang, Intrinsic Exciton-Phonon Coupling and Tuning in $\mathrm{Zn}\mathrm{Te}$ Nanowires Probed by Resonant Raman Scattering. *Physical Review Applied* **13**, 011001 (2020).

[4] C. Hu, Q. Chen, F. Chen, T. H. Gfroerer, M. W. Wanlass, and Y. Zhang, Overcoming diffusion-related limitations in semiconductor defect imaging with phonon-plasmon-coupled mode Raman scattering. *Light: Science & Applications* **7**, 23 (2018).

[5] T. Park, Y.-J. Guan, Z.-Q. Liu, and Y. Zhang, In Operando Micro-Raman Three-Dimensional Thermometry with Diffraction-Limit Spatial Resolution for GaN-based Light-Emitting Diodes. *Phys. Rev. Appl.* **10**, 034049 (2018).