Understanding Fundamental Limitations of Materials to Enable Advanced Design

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ABSTRACT

Future and advanced sensor technologies needed for DoD applications will require more efficient semiconductor materials and devices. Pushing sensor device performance beyond present levels requires a deep understanding of the fundamental limiters. Therefore fundamental research is needed to assure transition of technology from demonstration to system deployment. To address this problem, the Army Research Laboratory (ARL) and Boston University (BU) have come together to create a BU led Consortium for semiconductor Modeling of Materials and Devices (CSM). The Consortium brings together government, academia, and industry in a collaborative fashion to continuously push semiconductor research forward to meet DoD needs. The leveraged attributes of the Consortium include combined broad knowledge base in semiconductor modeling, materials growth and device expertise; sharing of computational resources; project continuity; and extension of the bench. Details regarding the Consortium's first research topic on understanding vertical transport in Type 2 SL will be discussed.

Keywords: semiconductors, modeling, semiconductor modeling center (CSM).

1.0 INTRODUCTION

The Army Research Laboratory (ARL) has established the Center for Semiconductor Modeling of Materials and Device Modeling[1-3] (CSM) to gain fundamental understanding of materials characteristics, and of device operation. CSM is designed to foster and accelerate collaborative research in the multi-scale modeling of semiconductor materials and devices, iteratively validated by experiments. The CSM brings together academia, industry and government labs, in the context of ARL's Open Campus Initiative[4], a key component of ARL's portfolio. ARL took the lead for developing CSM capability realizing that a combined group effort is the most efficient way to develop niche semiconductor technologies and products of DoD relevance. The ongoing collaboration between ARL and Boston University (BU) in the areas of photon detectors and emitters, and power devices has led to novel simulation tools that have made it possible for ARL to increase its modeling efforts, specifically in the more focused area of infrared detection.[5-7]

The structure of the CSM incorporates lessons learned from the successful implementation of ARL's Center of Research on Extreme Batteries (CREB) [8-9] that was stood up to foster and accelerate collaborative research in advanced battery materials and technologies, especially for extreme performance, environments and applications. The CSM was established in Phase 1, where the BU led CSM Consortium is being kicked-off in Phase 2 (see Figure 1).

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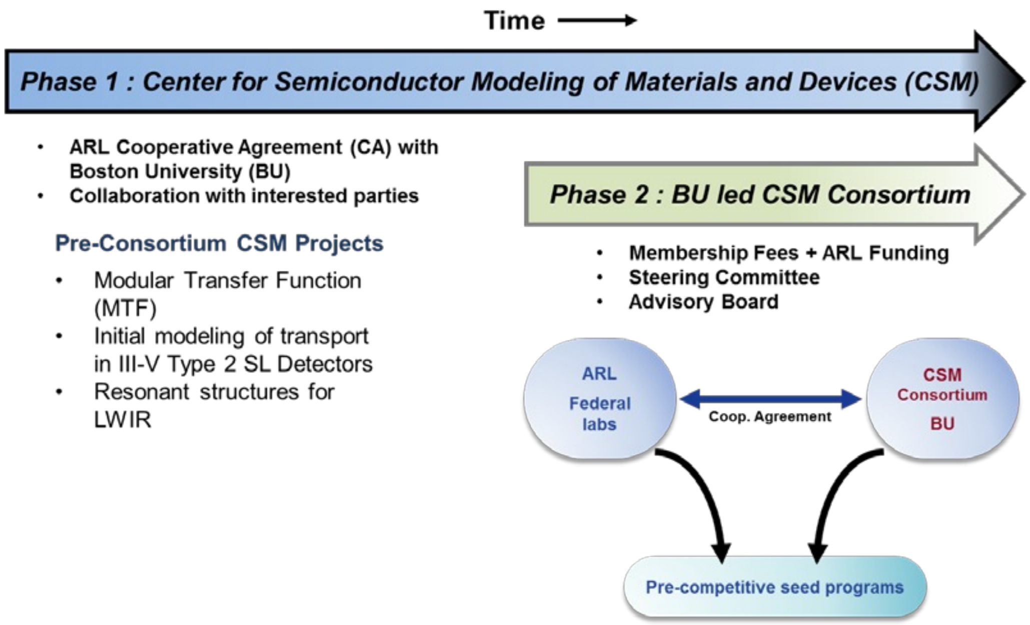

Figure 1. CSM and BU-led CSM Consortium Structure. Details for joining the CSM Consortium can be found at http://www.bu.edu/csm/

During Phase 1, ARL has been establishing legal agreements with BU, collaborating on pre-consortium research projects and working with BU and the CSM Steering Committee on creating the foundation for the CSM Consortium. In Phase 2, BU in collaboration with ARL, will kick-off the CSM Consortium and start building membership and exploring other funding opportunities for pre-competitive research projects.

Section 2.0 describes the status of an ongoing CSM project focused on understanding vertical transport in III-V Type 2 Superlattices. Section 3.0 highlights launching of the CSM Consortium. Section 4.0 touches upon a few envisioned next CSM projects. Section 5.0 is a summary of this paper.

2.0 VERTICAL TRANSPORT IN III-V TYPE 2 SUPERLATTICE (SL) STRUCTURES

The incumbent technology for the fabrication of LWIR infrared focal plane arrays (IRFPA), as well as future 3rd Gen innovations is based on the II-VI material system $Hg_{1-x}Cd_xTe$ grown on lattice matched CdZnTe substrates. However, significant investments by the DoD, are being made to displace the incumbent and exploit the use of III-V Type 2 SL materials for high performance cryogenically cooled IRFPAs.[10]

At this stage of development however, III-V Type 2 material systems such as Ga containing InAs/GaSb and Ga- free $InAs/InAs_{1-x}Sb_x$ SLs are limited by Shockley-Read Hall (SRH) defect centers of unknown origins with energy levels in the forbidden energy gap. The p-Type 2 InAs/GaSb SLs are limited by relatively low (~35 ns) minority SRH lifetimes. The measured hole minority carrier lifetimes for Ga-free n-Type 2 $InAs/InAs_{1-x}Sb_x$ SLs are >400ns[11] for LWIR and 9μs[12] for LWIR materials. These observations essentially shifted the efforts to n-Type 2 InAs/InAsSb SLs using nB_nn barrier designs to suppress the GR SRH dark currents; still the dominant current component.[13]

While significant progress has been made in the LWIR device fabrication/characterization, component integration and camera demonstration[10], the corresponding important material properties (hole minority carrier lifetime, fundamental absorption in the vicinity of the energy gap, and the vertical minority carrier diffusion length) of LWIR n-Type 2 $InAs/InAs_{1-x}Sb_x$ SLs are not well understood. Of great concern is low vertical mobility of holes, resulting possibly from transport via hopping between band tail localized hole states.

The approach we have chosen to investigate carrier transport in Type 2 SLs is a multiband k·p model coupled with the Non-Equilibrium Green's Function (NEGF) formalism. Based on a quantum field theoretical approach to non-equilibrium statistical mechanics, NEGF is a powerful tool to study carrier transport properties in nanostructures beyond the semi-classical limit: by treating carrier transport and recombination processes on the same footing, these tools will enable the modeling of modern and future optoelectronic devices. In superlattice absorbers, both absorption and transport are mediated by the superlattice states. The built-in or applied field has a strong influence on the transport regime, which ranges from miniband transport close to flat band conditions to Wannier-Stark hopping in the case of strong fields. Miniband conduction models are based on scattering transitions between delocalized Bloch states computed in the absence of any electric field. When, in realistic conditions, an applied or internal electric field is present, the electron wave functions become localized in the wells if the potential energy drop across a superlattice period exceeds the miniband width, i.e., the miniband breaks up in a ladder of localized quasi-bound states centered in the wells. In this situation, transport is only possible via an inelastic scattering process and is best described by hopping. In weakly coupled superlattices (at moderate electric fields), one has an intermediate regime in which transport is due to sequential tunneling of carriers from one well to the next, followed by relaxation by phonon emission. The NEGF formalism allows for enhanced representation of the physical processes of a multilayer structure that avoids a priori assumptions of the nature of the transport.

We report here the progress that we made in the development of the NEGF code with application to carrier transport in Type 2 InAs/GaSb superlattices (T2SLs). Our approach extends our rigorous 8-band k·p[14] model to zincblende crystals. Having introduced the correct operator ordering to ensure numerical stability, and having applied the axial approximation so that the band structure depends only on the transverse wavenumber |k|, we have diagonalized the 8×8 Luttinger-Kohn Hamiltonian into two decoupled 4×4 upper and lower Hamiltonian matrices (which include the conduction band (CB), the heavy-hole (HH), the light-hole (LH), and the spin-orbit split-off (SO) bands, for each spin), which is particularly important in the NEGF implementation because it significantly reduces memory requirements. Finally we have introduced this compact 4×4 k·p model in our NEGF code.

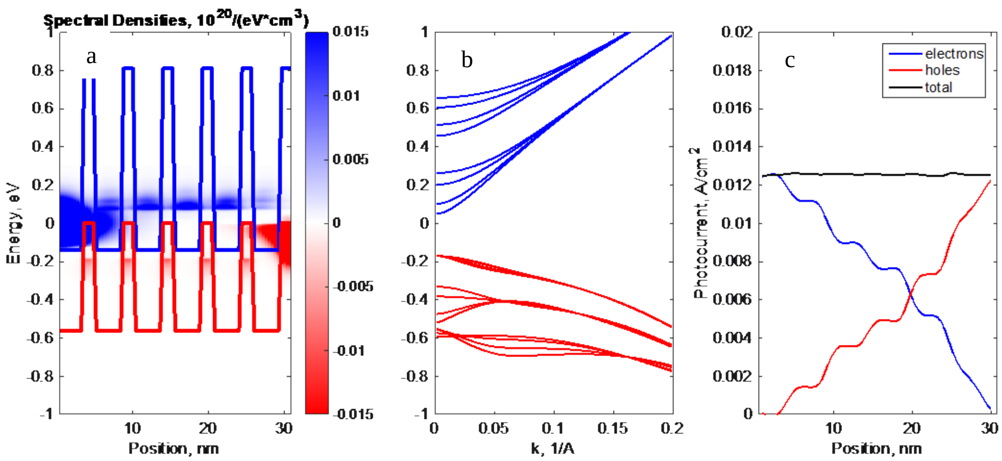

Figure 2. (a) Spectral carrier densities of a five-period InAs/GaSb superlattice at zero bias, illuminated with monochromatic light with photon energy 0.3eV and an intensity of $1kW/m^2$. (b) The corresponding subband dispersion as a function of the transverse wavenumber k. (c) Photocurrent integrated over energy and momentum.

The NEGF code includes acoustic scattering in the equipartition approximation, inelastic polar optical scattering, carrier-photon scattering, impurity scattering, and carrier-photon scattering. All self-energies are fully nonlocal and computed in the self-consistent Born approximation (SCBA). With this tool, we have obtained preliminary results of carrier transport in Type 2 InAs/GaSb superlattice absorbers illuminated with monochromatic light. Fig. 2 shows the extraction of carriers photogenerated and transported by the states of a five-period superlattice. The structure is uniformly illuminated by a mono-chromatic photon energy 0.3eV and an intensity of $1kW/m^2$. The SL structure is designed for a cut-off wavelength of 5.6μm. The electronic structure of the SL is presented in the center panel of Fig. 2, where the valence and conduction energy subbands are clearly visible. The left panel of Fig. 2 presents the calculated carrier, electrons in blue and holes in red, spectral densities. As it can be seen electrons are collected at the left contact and holes are the contact on the right of the device. In the same figure, the different populations of the first two conduction subbands can be clearly seen. On the other hand, holes only populate the heavy hole subband. The right panel of Fig. 2 presents the calculated electron (blue line) and hole (red line) current density in the structure. Upon convergence, the total current (electron + hole) is approximately conserved over the whole device region (black line). Convergence is achieved after ~ 100 inner iterations, this quantity strongly depends on the device size. We are currently considering more realistic structures consisting of superlattice absorbers embedded in PIN junctions. Additional work is needed to understand the role of inelastic processes in the transition from miniband to sequential tunneling transport.

3.0 CSM CONSORTIUM

Boston University is forming a consortium (**CSM Consortium**) aimed at advancing the state of the art in semiconductor materials and devices modelling. The consortium will work together with the Center for Semiconductor Modelling (**CSM**) recently formed at ARL. BU will soon kick-off the CSM Consortium and start building membership and exploring other funding opportunities for pre-competitive research projects.

The CSM Consortium Goals include:

- Bring together government, academia, and industry in a collaborative fashion to address research opportunities.
- Collaborate with diverse group of scientists to accelerate the development of a novel design approach to improve the ability of the science and technology community to develop novel semiconductor devices and transition into specific system applications.
- Develop robust and predictive models to minimize risk in developing new technology. The Consortium will focus on the theory, simulation and the experimental validation of the models.
- Exchange researchers between Consortium members to facilitate the execution of joint research projects.
- Provide educational programs to foster scientific interchange and facilitate transition of new technologies within the technology community.
- Provide access to unique infrastructure at member organizations.

Benefits of the CSM Consortium membership include:

- Group common understanding of the research needs and priorities
- New ideas and collaborators with expertise in multiple disciplines to solve problems
- Introduction and access to research, computation and production facilities of all member organizations
- Teaming to form joint proposals to target and capture external funding
- Joint publications
- Access to IP generated by CSM funding

Membership in the Consortium will be open to individuals, national and defense labs, universities and industry through membership via BU. Government partnerships can be established with the CSM Consortium directly through various contracting vehicles or through ARL’s contracting mechanism via a Memorandum of Agreement (MOA) while industry and academic partnership will be through the BU CSM Consortium. The CSM Consortium will be formalized via membership agreements (MA) and Articles of Collaboration (AOC)[15]. The CSM Consortium steering committee, aided by the CSM Advisory Board, will be responsible for selection and funding of the projects.

4.0 ENVISIONED NEXT CSM PROJECTS

Under discussion are several subjects of interest that the CSM is considering as projects to pursue. A few of them are briefly described in this section.

HOT (High Operating Temperature) HgCdTe

Theoretically, the operating temperature of HgCdTe photodiodes could be raised significantly. Developments in HgCdTe material (very low doping and defects, excellent bandgap profile control, etc.) & modeling (detailed 3D device and advanced materials models) make ***doubling the BLIP FPA Top*** a realistic goal.

We propose to establish validated predictive models for HOT MCT including materials, device, and system optimization. The expected outcomes of the project are validated understanding of device design for HOT detectors; band gap and doping profiles, grown and/or implanted junctions, Isotype barrier structures, radiative as well as Auger suppression, resonant structures, cross-talk and other key parameter analysis.

Our approach includes using Synopsys based heterojunction model to design HOT structures, fabricate and comparing structures using PEC and Banded FPAs, and iterating to improve design based on measurement/analysis of devices. The project payoff is to greatly improve the operating temperature of high performance IR detectors and realizing the associated reduction in system cost.

Excess Noise Reduction

HgCdTe operating temperature exceeds any other IR material for median devices, but excess noise (e.g. 1/f, blinkers) limits operability forcing lower operating temperature. Recent HgCdTe technology and materials/diode modeling have matured enough to address/explore noise inducing defects in order to eliminate them.

The proposed project would be to simulate/predict excess noise from trapped charge plus tunneling in defects, compare with FPA results, and iterate/refine both model and device to validate model and reduce noise. The proposed approach is to first model HgCdTe device I-V, spectral response and compare with actual device data to assure good description of median behavior. Then model extended defects, by including in device model localized trapped charge (on inclusions, clusters, dislocations, etc.) with varying magnitude and location in the depletion region. The model understanding will be validated based on FPA measurements of current devices. The architecture will be modified to reduce defects and their effect based on model results – fab/test FPAs, validate, iterate. The expected project outcomes would be: validated understanding of primary sources of excess noise (electrical models, physics/material models), design and fab modifications that reduce excess noise verified by FPA test, higher operability and greater correction stability of all HgCdTe FPAs, especially HOT FPAs – reducing the need for cooling to improve operability and stability, and potential applicability to all IR photodiode imagers.

5.0 SUMMARY

Given DoD interests in III-V Type 2 SLs technologies as an alternative to the incumbent technology, which is based for LWIR and VLWIR on II-VI HgCdTe alloy semiconductor, it is timely for CSM to focus on the basic properties of Type 2 $InAs/InAs_{1-x}Sb_x$ SLs, in particular the transport properties associated with this material system. The results of the pre-consortium research efforts presented here are a first step towards developing validated models needed for further advancement of LWIR III-V Type 2 SLs. The CSM Consortium aims at bringing together the expertise and capabilities of Industry, Academia and other government agencies in a collaborative fashion to accelerate this research to insure timely transitions to the soldier. While the CSM and CSM Consortium have decided to start with IR materials, we intend to expand the research activities to other semiconductor materials and devices. These future efforts will be based on DoD needs and community interest.

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REFERENCES

[1] Perconti, P., Alberts, W. C. K., Bajaj, J., Schuster, J. and Reed, R., "Sensors, Nano-Electronics and Photonics for the Army of 2030 and Beyond", Proc. SPIE 9755, 975506 (2016).

[2] Philip Perconti, Sarah S. Bedair, Jagmohan Bajaj, Jonathan Schuster, and Meredith Reed, "Center for Semiconductor Materials and Device Modeling: Expanding Collaborative Research Opportunities between Government, Academia, and Industry", Proc. SPIE 9933, 993308 (2016).

[3] Jagmohan Bajaj, Roger DeWames, Jonathan Schuster, Meredith Reed, Phil Perconti, and Enrico Bellotti "Accelerating Technology Innovations by Early Understanding of Fundamental and Technology Limitations of Material Synthesis and Device Operation", SPIE Proceedings, vol. 10111, pp. 10111-10117, 2017.

[4] http://www.arl.army.mil/opencampus/

[5] Bellotti, E., Schuster, J., Pinkie, B., and Bertazzi, F., "Multi-scale modeling of photon detectors from the infrared to the ultraviolet," Proc. SPIE 8868, 88680R-1-8 (2013).

[6] Schuster, J., DeWames, R.E., DeCuir Jr., E.A., Bellotti, E., Dhar, N., and Wijewarnasuriya, P.S., "Heterojunction depth in P+-on-n eSWIR HgCdTe infrared detectors: generation-recombination suppression," Proc. SPIE 9609, 960904-01-11 (2015).

[7] Schuster, J., DeWames, R.E., DeCuir Jr., E.A., Bellotti, E., and Wijewarnasuriya, P.S., "Junction optimization in HgCdTe: Shockley-Read-Hall generation-recombination suppression," Applied Physics Letters, 107, 023502-1-5 (2015).

[8] Eric Wachsman, Cynthia Lundgren, Esther Takeuchi, Kang Xu, Chunsheng Wang, Joseph Dura, David Jacobson, Kahlil Amine and William Acker, "The Center for Research on Extreme Batteries", The Electrochemical Society Interface, Fall 2016.

[9] http://creb.umd.edu/

[10] http://www.cerdec.army.mil/news_and_media/Army_holds_showcase_of_infrared_technology_advancements/

[11] S. P. Svensson, D. Donetsky, D. Wang, H. Hier, F. J. Crowne, and G. Belenky, J. Cryst. Growth **334**, 103 (2011).

[12] B. V. Olson, E. A. Shaner, J. K. Kim, J. F. Klem, S. D. Hawkins, L. M. Murray, P. Prineas, M. E. Flatte, and T. F. Boggess, Appl. Phys Lett. **101**, 092109 (2012).

[13] DeWames, R. E., "Opto-electronic properties of mid-wavelength: n Type II InAs/$InAs_{1-x}Sb_x$ and $Hg_{1-x}Cd_xTe$," Journal of Electronic Materials 45(9), 4697-4704 (2016).

[14] [Xiangyu Zhou, Francesco Bertazzi, Michele Goano, Giovanni Ghione, Enrico Bellotti, Deriving k· p parameters from full-Brillouin-zone descriptions: A finite-element envelope function model for quantum-confined wurtzite nanostructures, Journal of Applied Physics, Vol. 116, Issue 3, Pages 033709, 2014.

[15] http://www.bu.edu/csm/