Accelerating Technology Innovations by Early Understanding of Fundamental and Technology Limitations of Material Synthesis and Device Operation

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ABSTRACT

Timely technology transition with minimal risk requires an understanding of fundamental and technology limitations of material synthesis, device operation and design controllable parameters. However, this knowledge-based approach requires substantial investment of resources in the Science and Technology (S&T) stage of development. For low volume niche semiconductor technologies of Department of Defense (DoD) relevance, there is little drive for industry to expend their limited resources towards basic research simply because there is no significant return on investment. As a result, technology transition from S&T to product development is often delayed, expensive and carries risks. The Army Research Laboratory (ARL) is addressing this problem by establishing a Center for Semiconductor Modeling of Materials and Devices (CSM) that brings together government, academia, and industry in a collaborative fashion to address research opportunities through its Open Campus initiative. This Center leverages combined core competencies of partner organizations, which include a broad knowledge base in modeling, and its validation; sharing of computational, characterization, materials growth and device processing resources; project continuity; and 'extension of the bench' via exchange of researchers between affiliated entities. A critical DoD technology is sensing in the infrared (IR) spectrum, where understanding of materials, devices and methods for sensing and processing IR information must continually improve to maintain superiority in combat. In this paper we focus on the historical evolution of IR technology and emphasize the need for understanding of material properties and device operation to accelerate innovation and shorten the cycle time, thereby ensuring timely transition of technology to product development and manufacturing. There are currently two competing IR technologies being pursued, namely the incumbent II-VI $Hg_{1-x}Cd_xTe$ technology and the III-V Type 2 Superlattices (SLs) technology. A goal of the CSM is to develop physics based models for Type 2 SLs with the capability to timely understand the knowledge gap between what is built and what is designed.

Keywords: semiconductors, multi-scale modeling, semiconductor modeling center (CSM), sensors, infrared (IR), HgCdTe, III-V Type 2 SL, photonics, nBn, XBn, pBp.

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1.0 INTRODUCTION

The General Accounting Office (GAO) generated a Best Practices Report[1] in 1999 confirming that failure to properly mature new technologies in the science and technology (S&T) phase consistently contributes to cost and schedule over-runs in the acquisition of weapons systems. This report states "maturing new technology before it is included on a product is perhaps the most important determinant of the success of the eventual product or weapon system." As a best practice, it also states that technology development and product development should remain exclusive. Therefore, it is incumbent upon both S&T and product managers to ensure that a technology is mature before including it as part of a weapons system. A 2004 GAO Best Practices Report[2] proposed a knowledge-based approach that uses "knowledge-points" shown in Figure 1 as the key identifiers used as go or no-go metrics to separate the different stages of the development process. This is analogous to a stage-gate model proposed by Bigwood[3], where the stages are the Technology Readiness Levels[1] (TRL) and the gates are the knowledge points that determine what stage (TRL) the technology resides. For instance, a knowledge point in transitioning from TRL 6 to TRL 7 could be the existence of robust and predictive materials and device models that provide quantitative information on the operation of the semiconductor device, i.e. "can we build what we design?"

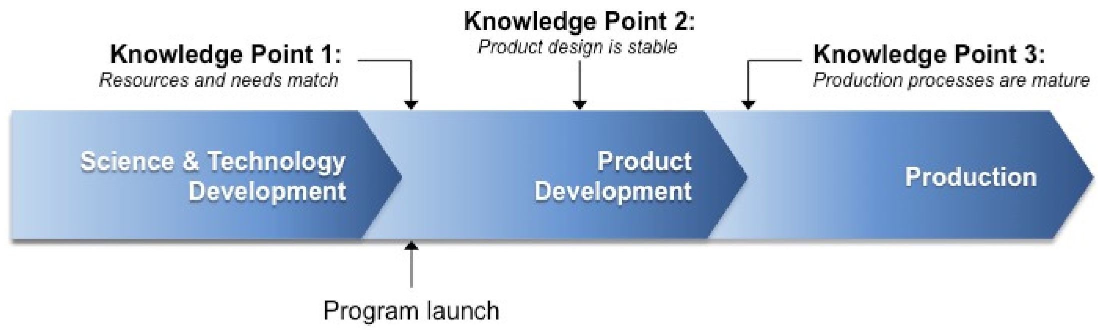

Figure 1: Adaptation of the knowledge-based approach recommended by the Government Accounting Office (Ref 2).

The Army Research Laboratory (ARL) has established the Center for Semiconductor Modeling of Materials and Device Modeling[4-6] (CSM) to bridge the gap depicted in Figure 2. CSM is building the capability to simulate real devices, with a goal to clearly differentiate what is deterministic (output of mathematical equations) and randomness of the device metric, leading to less variance, minimal randomness, and stable device design.

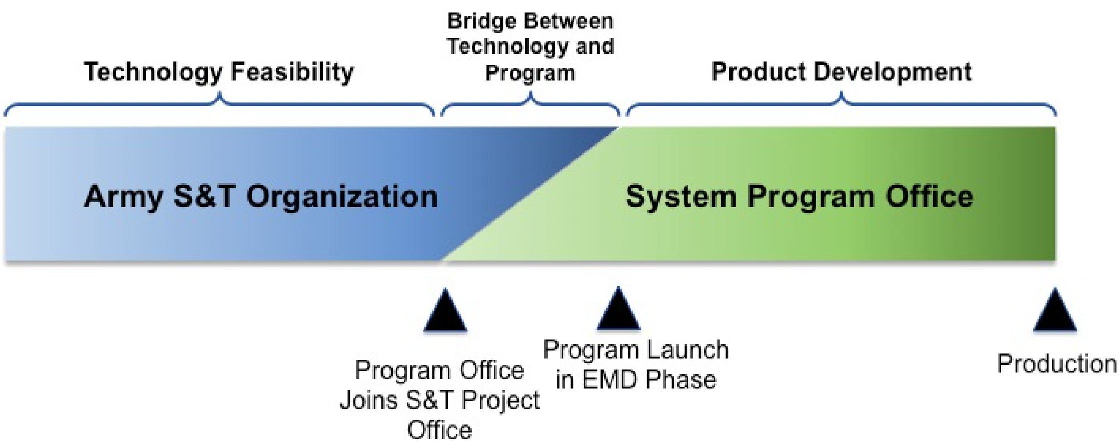

Figure 2: Technology development and transition to product/system.

The CSM brings together academia, industry and government labs, in the context of ARL's Open Campus Initiative[7], that has become a key component of ARL's portfolio. Section 2.0 describes the Open Campus Initiative. Section 3.0 describes the Center for Semiconductor Modeling of Materials and Devices (CSM) set up to accelerate innovation and shorten the associated cycle times. Also included in this section are the status of the Center and the next steps. Section 4.0 highlights the initial CSM focus on infrared (IR) materials and devices. Section 5.0 is a summary of this paper.

2.0 OPEN CAMPUS INITIATIVE

The Open Campus initiative[7] of the ARL is a collaborative endeavor (see Figure 3), with the goal of building a science and technology ecosystem that encourages groundbreaking advances in basic and applied research areas of relevance to the Army. This Open Campus approach is aimed at altering the typical research and development paradigm by removing physical and procedural barriers traditionally inhibiting efficient collaborative interactions between government laboratories, industry and academic partners. Through the Open Campus framework, partners can work directly with ARL researchers and share ARL's specialized research facilities. Likewise, ARL researchers can work at partner institutions, bringing with them unique knowledge and perspectives about Army-specific problems, other government research funding opportunities, and providing increased access to the broader DoD research and acquisition community. The goal of Open Campus is to foster cutting-edge, Army-relevant fundamental research in a collaborative environment for the benefit of all partners.

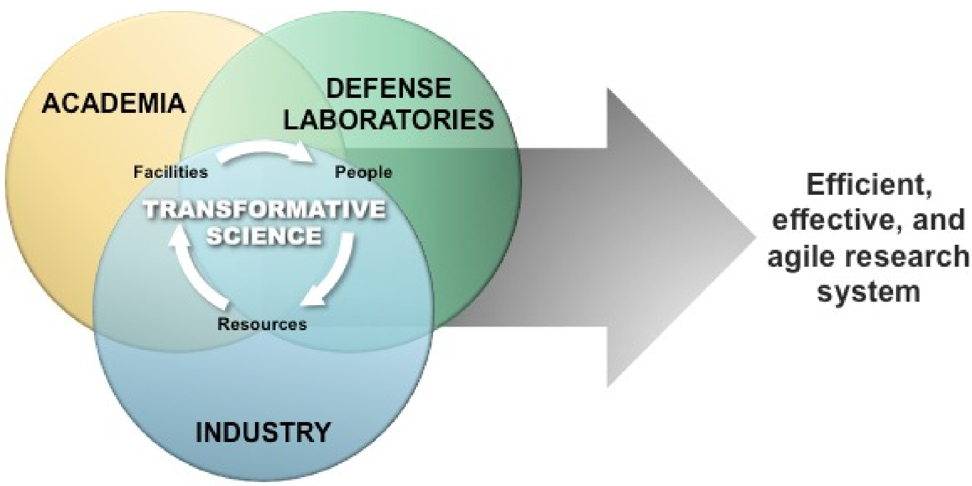

Figure 3: ARL's Open Campus Initiative fosters collaborative partnerships between industry, academia and government labs.

The tools available to aid the laboratory in its collaborative endeavors through Open Campus include Cooperative Agreements (CA), Educational Partnership Agreements (EPA) and Cooperative Research and Development Agreements (CRADA). CAs are tools that are used when parties wish to work together on the same project while sharing each party's expertise, facilities and equipment. These agreements require government involvement and while funds may be passed from the government to the partner, the partner may not provide money to the federal partner. CRADAs are formal agreements between one or more federal laboratories and one or more non-federal parties under which the government provides personnel, facilities, equipment or other resources. Under a CRADA, ARL may receive financial contributions, but funds may not be sent to the partner.

The Open Campus Initiative has led to the formation of several Open Campus Centers, focused on specific areas, bringing together academia, industry, and government to apply their respective scientific strengths on innovative research that benefits the members of each center. As an example, the goal of the Center for Research on Extreme Batteries (CREB)[8-9] is to foster and accelerate collaborative research in advanced battery materials, technologies and characterization techniques with a focus on batteries for extreme performance, environments and applications, such as those needed for the defense, space, and biomedical industries. The concept grew out of a partnership between ARL and

University of Maryland (UMD), with the addition of National Institute of Standards and Technology (NIST) and NY BEST (see Figure 4). The CREB Steering Committee consists of members from each of these organizations. UMD has established a separate non-profit organization, the CREB Consortium, administered by UMD, as a mechanism to participate in activities associated with CREB and to foster collaboration between Federal labs and academic/industrial partners. Membership in the CREB Consortium is open to individuals, national and defense labs, universities, and industry through tiered membership fees.

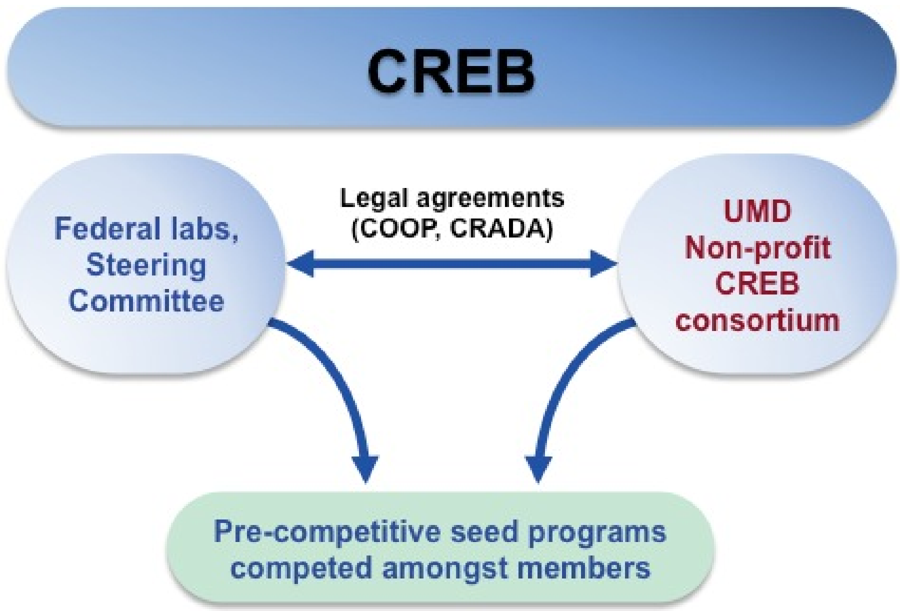

Figure 4: Diagram of the CREB structure.

3.0 CENTER FOR SEMICONDUCTOR MODELING OF MATERIALS AND DEVICES

The concept to create a Center for Semiconductor Modeling of Materials and Devices (CSM) grew out of ongoing partnership between ARL and Boston University (BU) as a part of the Enterprise for Multiscale Research of Materials (EMRM). The EMRM program is focused on the design and development of new materials for the Army, expanding ARL's core campaign in materials research, developing a computational materials-by-design perspective for the next generation of government, academic, and industry scientists, and fostering innovation through increased collaboration.

EMRM[10-12] is developing the underpinning scientific foundation and design tools to enable the modeling, design, analysis, prediction, and behavioral control of novel materials, and exploring material interactions from atomistic to continuum in both temporal and spatial scales, under extreme conditions, and in the presence of defects, surfaces, and interfaces within the materials. Within the EMRM, the Alliance for Computationally-guided Design of Energy Efficient Electronic Materials (CDE3M) has been developing validated models for electronic materials across multiple scales and collaborating with ARL on experimental characterization, materials synthesis and processing. Key to the CDE3M success is the ARL's state-of-the-art computational and experimental facilities that play a key role in enabling the development of these shared simulation models. The collaboration between ARL and Boston University (BU), in the areas of photon detectors[13] 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 using HgCdTe devices.[14-15]

The goal of the CSM is to foster and accelerate collaborative research in the multi-scale modeling of semiconductor materials and devices, iteratively validated by experiments. This Center brings together leveraged core competencies that exist at government, academic and industrial institutions. The leveraged attributes of the Center include combined broad knowledge base in semiconductor modeling; combined modeling, materials and device expertise and availability; sharing of computational resources; project continuity; and "extension of the bench" via exchange of researchers between affiliated entities. ARL is pushing for the CSM capability realizing that a combined group effort is the most efficient way to develop niche semiconductor technologies and products of DoD relevance.

The intent of the CSM is to simulate real materials and devices in real environments, understand what limits the technology, understand the parameters that control the performance, eliminate variances to the maximum extent possible and arrive at a materials and device design which will reproducibly yield the projected performance. Doing so at an early stage of innovation will undoubtedly lead to acceleration toward the next disruptive innovation. This acceleration is becoming increasingly important because the environment is changing rapidly and to stay ahead we must innovate faster.

We are modeling the structure of CSM by incorporating lessons learned from the successful implementation of the CREB described earlier in Section 2.0. The CSM has been established in Phase 1, to be followed by the BU led CSM Consortium in Phase 2 (see Figure 5).

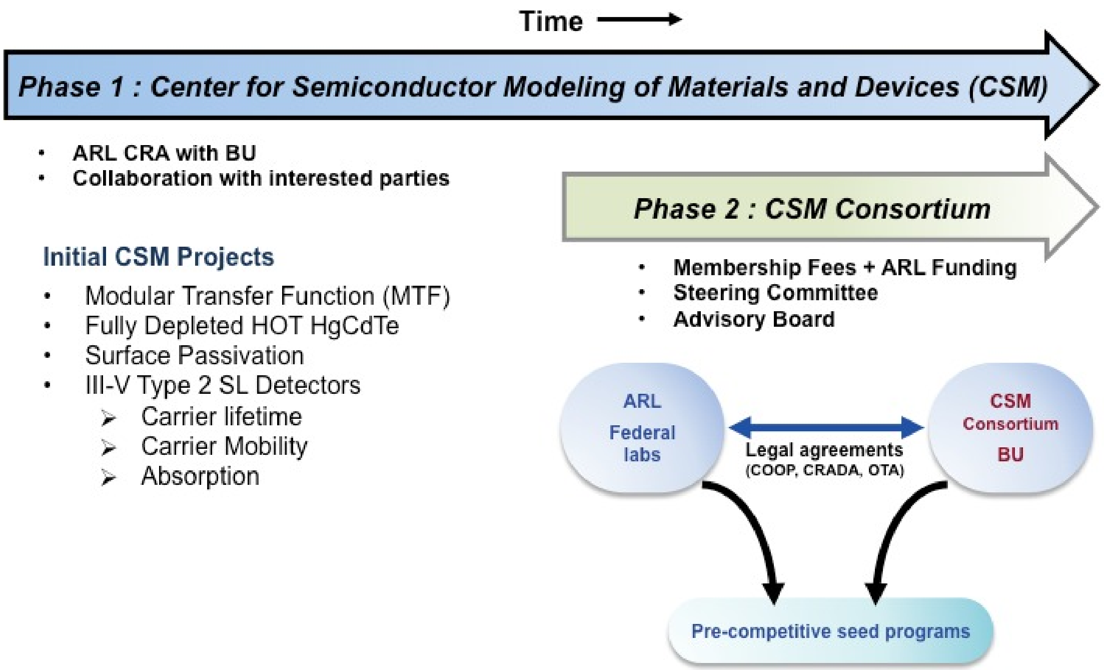

Figure 5. CSM structure.

During Phase 1, ARL is 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 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, 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 encompass membership agreements, steering committee and advisory board, and will fund pre-competitive seed projects. Until the CSM Consortium is established, the Center activities will continue with BU and through CRADAs with interested industrial partners.

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

The initial focus of the CSM is on IR materials and devices, with the vision of broadening the scope in due time to include other semiconductor systems, such as visible sensors, ultraviolet (UV) sensors and emitters, power electronics, etc.

4.0 IR – CSM

Figure 6 captures the historical[16] evolution of IR technology innovations, highlighting key developments that led to several generations of IR imaging sensors. Advances in HgCdTe materials and devices enabled the development of three generations of detector devices. The first disruptive innovation led to the 1st Gen Photoconductive HgCdTe Common Module program. The early 1st Gen devices utilized HgCdTe linear arrays in which an individual electrical contact made to each element of a cooled multi-element focal plane array (FPA) is brought out to an individual electronic channel at ambient temperature. The first generation scanning system does not include multiplexing functions in the FPA. Developments in photovoltaic junction detectors, readout circuitry and indium-bump hybridization led to the next disruptive innovation leading to 2nd Gen two-dimensional staring hybrid FPAs. The advent of MBE HgCdTe and associated bandgap engineering capability allowed two-color staring FPAs, paving the way to currently ongoing Engineering and Manufacturing Development (EMD) phase of the 3rd Gen IR forward looking infrared sensors for vehicles. Each generation of sensors has been providing significant improvement in application capability over the previous one, with the 3rd Gen sensors designed to enable detection, recognition and identification of targets with increased clarity and at significantly longer ranges.

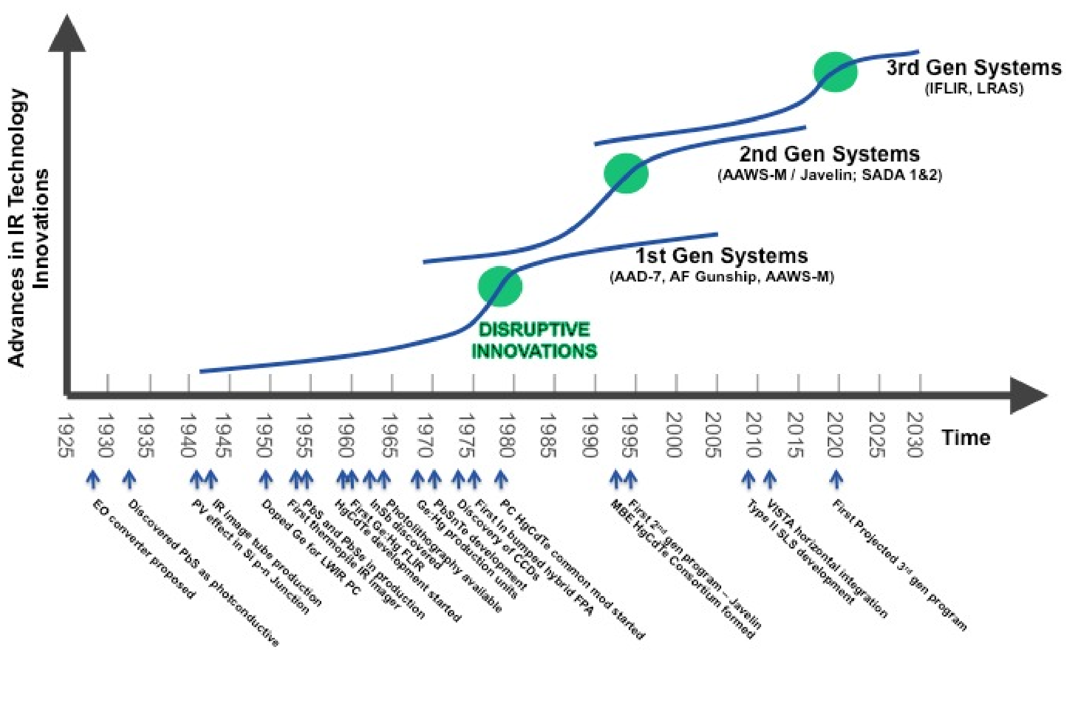

Figure 6: Historical evolution of Infrared Technology Innovations.

Evident from Figure 6 are long (15 - 20 years) innovation cycles and long (>25 years) product life cycles. There are several factors that can contribute to these long times. However, from a technology standpoint it is the insufficient knowledge and underestimation of technology risk when transitioning to product development that result in schedule delays, cost overruns and long innovation cycle times, as described in Best Practices GAO reports[17-18]. In particular, the report emphasizes that in successful commercial ventures, the accumulation of knowledge and the elimination of risks or unknowns are completed well before production units are made. The report also points out that in the DoD acquisition process, a clear distinction is not made between technology development and product development, and product development programs are launched in the technology development phase with the hope that risk reductions and closing knowledge gaps can be managed in the product development stage. Based on GAO lessons learned, often this strategy results in cost overruns, delays, life cycle cost increase and overall process randomness; basically the process is not in control nor stable, resulting in products of inferior quality and performance less than what was originally intended.

For future 3rd Gen innovations, there are currently two competing technologies being pursued. One is based on the incumbent II-VI HgCdTe and the other is based on the III-V Superlattice (SL) materials. A goal of the CSM is to develop physics based models for Type 2 SLs with the capability to timely understand the nature of the knowledge gap between what is built and what is designed. This will serve as a metric in the S&T stage to assess the technology readiness level and maturity of this IR technology.

4.1 III-V Type 2 Superlattice (SL) Technology

The incumbent technology for the fabrication of LWIR and VLWIR infrared focal plane arrays (IRFPA) is based on the II-VI material system $Hg_{1-x}Cd_xTe$ built 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.[19] Theoretically, the III-V Type 2 SL "defect free" structures possess several potential advantages over LWIR and VLWIR HgCdTe alloy material for use in infrared photodetectors.[20] In particular, (1) their electronic bands can be engineered to suppress Auger recombination relative to that in comparable bulk detectors; (2) the band-to-band tunneling currents are lower than those in comparable bulk detectors due to greater effective masses in the growth-axis direction. The energy band of a "defect free" semiconductor is essentially that of an impurity semiconductor with shallow donor or acceptor band gap states occupied by conduction electrons and holes respectively. In this picture the density of states curves in both the conduction band and valence band go to zero at the band edges.

However, real III-V Type 2 material systems such as InAs/GaSb and $InAs/InAs_{1-x}Sb_x$, known as Ga containing and Ga- free III-V SLs respectively, are limited by Shockley-Read Hall (SRH) defect centers of unknown origins with energy levels in the forbidden energy gap. It is important to note that the p-Type 2 InAs/GaSb LWIR technology as practiced by SCD, Israel has transitioned into the stages of product development and manufacturing.[21]

Known[22-23] is that in conventional shallow $n^+p^-p^+$ homojunction photodiode fabricated from III-V Type 2 InAs/GaSb SLs, the dark currents are dominated by generation-recombination (GR) recombination processes originating in the depletion region of the device. This study[22-23] measured current density at a reverse bias of -50mV as a function of the inverse temperature for an $n^+p^-p^+$ device with band gap energy of 0.121 eV at 0K, and area = 1.34×10^{-5} cm^2 and an absorber layer (AL) thickness of 2.3μm. It was concluded that in the temperature region > 100K the dominant current is the diffusion current, for temperature < 100K the dominant current is the GR component and at temperature < 50K, the dark current is limited by trap assisted tunneling. The reported GR current density at 77K is 5×10^{-4} A/cm^2, whereas the diffusion current density is 5×10^{-5} A/cm^2.

Obviously desired is diffusion-limited behavior all the way, and commonly used for this purpose for III-V Type 2 SLs are barrier detectors.[24] Klipstein[21] compared the dark current as a function of temperature of LWIR pB_pp barrier device (consisting of InAs/GaSb T2SL absorber and contact layers, and a InAs/AlSb T2SL barrier layer) with that of a standard LWIR n-on-p diode based solely on an InAs/GaSb Type 2 SL. The study reported that the barrier device is diffusion limited down to 77K where the dark current is reduced by x20 compared to the GR limited dark current of the n-on-p diode. An important observation is that the magnitude of the GR current density they measured on their diode is comparable with the GR current density component for the $n^+p^-p^+$ homojunction diode[22]. Likewise, the diffusion component measured on the heterojunction barrier device is comparable to the diffusion current of the $n^+p^-p^+$ diode[22-23]. The implication is that the 35 ns minority carrier lifetime obtained from the analysis of individual relatively large $n^+p^-p^+$ homojunction device data has not been improved. This is probably not surprising given that studies of MWIR InAs/GaSb SLs suggest that a defect native to GaSb may be responsible for creating a large number of recombination centers that limit the minority carrier lifetime.[25] The 35ns electron minority carrier lifetime also explains the FPA data reported.[21] The 77K dark current density measured on pB_pp barrier detectors is a factor of 50 lower than the dark current density predicted for $Hg_{1-x}Cd_xTe$ by Rule-07.[26] Hence from a BLIP performance perspective the p Type2 InAs/ GaSb SL barrier detector will need to be significantly cooled to lower temperature to achieve the same $J_{dark}/J_{photon} \approx 0.2$ BLIP condition. For high flux conditions, however, the performance may be adequate.

In contrast to the p-Type 2 InAs/GaSb SLs limited by relatively low (~35 ns) minority SRH lifetimes, the measured hole minority carrier lifetime for a Ga-free LWIR n-Type 2 $InAs/InAs_{1-x}Sb_x$ SLs is greater than 400ns[27], and 9μs in a MWIR n Type 2 SLs[28]. 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.[29]

However, optical measurements[30] of vertical carrier mobilities of MWIR InAs/GaSb SLs suggested that the relatively high electron mobility is indicative of miniband transport in extended states, and that the very low hole mobility is indicative of the hole states being localized and transport occurring via hopping. Localization also appears to describe states in MWIR InAsSb SLs as suggested by the blue shift of the photoluminescence peak.[31] For the case of the MWIR InAs/InAsSb it appears that interface disorder is responsible for the localization. Supporting this picture is the monolayer-by-monolayer analysis[32] of (46Å, 17Å) $InAs/InAs_{1-x}Sb_x$, x=0.33 SLs. The scanning tunneling microscopy (STM) images show substantial Sb disorder and Sb segregation.[33] Based on these observations of structural disorder and hole states being localized, a possibility is conduction between localized sates in band tails that merge into the extended conduction and valence band states.[34] The transport is a thermally activated process that involves tunneling between localized sates. These transport properties differ significantly from the equivalent crystalline transport properties and an expected implication of this would be decreasing quantum efficiency with decreasing temperature.

The III-V Type 2 SL optical absorption properties depend heavily on the physical structure of the SL as a whole. The individual layers in each period are composed of different materials of alternating energy band gaps. Varying the layer thicknesses comprising each period, the mole fraction of the ternary alloy, doping, and the number of periods all influence the absorption coefficient of the SLs and this must be modeled and optimized taking into considerations mismatch of the multilayer structure grown on GaSb substrate. In a recent publication[35] on interband absorption strength in LWIR Type 2 SL with small and large superlattice periods compared to bulk, the authors concluded that for the conventional LWIR SLs the absorption is much weaker than the bulk material with the same energy gap. This is because the electron-hole overlap in the conventional LWIR Type 2 SL occurs in the hole well which is significantly smaller than the thickness of absorbing layer. All of the above considerations point to the need for more in depth understanding of the material properties of Type 2 SLs, in particular the n-Type 2 $InAs/InAs_{1-x}Sb_x$ SL.

In summary it is evident that LWIR and VLWIR IRFPAs built from p-Type 2 InAs/GaSb as practiced by SCD, are not likely to displace HgCdTe for high performance large format small pitch arrays; this assessment is based on the 35 ns electron minority carrier lifetime. Modeling can contribute to identify microscopic defects that cause SRH lifetimes and in combination with experiments find paths to reduce or eliminate them; such activities however are likely to be very consuming.

Regarding the situation with the LWIR and VLWIR n-Type 2 SLs, $InAs/InAs_{1-x}Sb_{x,}$ while significant progress has been made in the LWIR device fabrication/characterization, component integration and camera demonstration[19], the corresponding important material properties are not well understood. For LWIR and VLWIR photodetectors, the most important basic properties are hole minority carrier lifetime, fundamental absorption in the vicinity of the energy gap, and the vertical diffusion length for the minority carriers. Of great concern, in particular for LWIR and VLWIR, where the content of Sb needs to be large, is the possibility that the transport in n-Type 2 $InAs/InAs_{1-x}Sb_x$ SL may be limited by band tail conduction. Urgently needed is data on the vertical mobility of holes, as extracted from the measurement of the quantum efficiently, and from direct measurements[36-37] to confirm or disprove the onset of transport via hopping between band tail localized hole states.

From the analysis of the data it will become evident what physical model will be needed to explain the quantum efficiency and the vertical carrier mobility. If the suggested form of the defect band gap state is that of a crystalline semiconductor, expected is that the drift- diffusion continuity equations used to model crystalline semiconductors will explain the data. However, if the suggested transport is via hopping, new modeling and simulation tools will need to be developed to determine root causes and determine whether the limitation is fundamental or technological. Lack of such knowledge, with significant unknowns, can translate into technology risks when transitioning from technology to product development.

To overcome limitations associated with holes as minority carriers, studies are ongoing to exploit p-Type 2 $InAs/InAs_{1-x}Sb_x$ SLs where electrons are minority carriers, hoping that the lifetimes remain in the range observed in n-Type2 $InAs/InAs_{1-x}Sb_x$ SLs.[38] A challenge is that the background doping is n-type, hence counter doping is required to convert the material to p-type. The authors[37] conclude that with Be doping, the lifetime is reduced at all temperatures and that needed is more in depth understanding of the causes of the reduced carrier lifetime.

5.0 SUMMARY

The GAO reports on "Best Practices" advocate a Knowledge Based Approach to improve weapon acquisition; separating technology development from product development and essentially developing and maturing technology before introducing it into product development. Based on the GAO studies for the cases studied that required more technical knowledge, at "Knowledge Point 1", technology risks were reduced, cost and schedules were improved, cycle time was reduced, and quality was improved during product development by gaining significant knowledge about a technology before launching the product development.

However, undermining this approach is the availability of resources needed in the S&T stage of development for DoD "niche" markets, where products are diversified and volumes are small. This situation is the case in the DoD needs of infrared sensors for future weapon systems. ARL initiated Center for Semiconductor Modeling is an organizational strategy to address the resources needed to mature technology in the S&T stage of technology development, thereby reducing technical risks. The timely idea is to establish partnerships with stakeholders in the government, industry and the universities who share a common interest in accelerating the innovation cycle and reducing the product life cycle. The concept was introduced in a workshop held at ARL in April of 2016 to discuss research needs, and further meetings were scheduled with industry. From these discussions it became evident that knowledge gaps existed in III-V Type 2 SLs technologies. 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.

A first step in getting started is to establish Status Quo to answer the important question: What "defect physics model" will be needed to simulate real materials and devices to understand the underlying physical concepts to enable a data based assessment of the real potential of the Type 2 SL technologies for LWIR and VLWIR high performance, large format, small pitch and affordable cryogenically cooled IRFPAs.

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