Sensors, Nano-Electronics and Photonics for the Army of 2030 and Beyond

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ABSTRACT

The US Army's future operating concept will rely heavily on sensors, nano-electronics and photonics technologies to rapidly develop situational understanding in challenging and complex environments. Recent technology breakthroughs in integrated 3D multiscale semiconductor modeling (from atoms-to-sensors), combined with ARL's Open Campus business model for collaborative research provide a unique opportunity to accelerate the adoption of new technology for reduced size, weight, power, and cost of Army equipment. This paper presents recent research efforts on multi-scale modeling at the US Army Research Laboratory (ARL) and proposes the establishment of a modeling consortium or center for semiconductor materials modeling. ARL's proposed Center for Semiconductor Materials Modeling brings together government, academia, and industry in a collaborative fashion to continuously push semiconductor research forward for the mutual benefit of all Army partners.

Keywords: sensors, nano-electronics, photonics, army applications, infrared (IR), soldier requirements

1. INTRODUCTION

The assured timely transition of technology from demonstration to product development to system deployment, with minimal cost and schedule risk requires good understanding of materials synthesis, device operation, and the design-controllable parameters. Ideally, performance of a given technology should be predictable from theoretical concepts that also yield diagnostic tools to illuminate the cause of a deviation from designed performance.[1] This understanding comes from reliable multi-scale modeling of devices, a capability that is currently being developed and exploited at ARL.

ARL, through its basic research in semiconductor materials and devices, is developing and refining capabilities that allow modeling, simulation, and experimental validation from the atomic-scale to the device-scale. One critical Army technology is sensing in the IR spectrum, which continues to be an extremely active area of research; materials and methods for sensing and processing of IR information must continually evolve to maintain overmatch of similar technologies possessed by potential adversaries. Thus, a key research area at ARL is in new materials and devices intended to increase the capability of IR sensors for Army applications. Part of this research involves the aforementioned multi-scale modeling to predict how a new material will perform across all spatial and temporal scales.

Multi-scale modeling continues to be a rich technical area with many separate academic, government, and industry entities performing similar research.[1-6] In an effort to provide the maximum benefit to all while sharing competencies and resources, ARL is pursuing a Center for Semiconductor Materials Modeling (the Center). The intent of this Center is to create a platform from which collaborative agreements can be initiated to further the mutual technological goals of the Army, academia, and industry. To this platform, ARL brings its diverse collaborative portfolio, which will be the launching point for collaboration among the various entities.

Section 2 presents a brief overview of multiscale modeling as it relates to the needs of the Army and presents an exemplar successful result from ARL's multi-scale modeling efforts in materials research. Section 3 discusses a collaborative initiative at the Army Research Laboratory, the Open Campus. Section 4 presents the Army's vision for a

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multiscale semiconductor modeling center including an assessment of how the proposed center will progress to meet anticipated future Army needs. The final section gives some concluding remarks.

2. OVERVIEW OF MULTISCALE MODELING AT ARL

The ARL Enterprise for Multiscale Research of Materials **(**EMRM) program is: transforming the approach used to design and develop 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 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. To be successful, the approach includes theory, validated modeling at and across multiple scales, experimentation, characterization, identification of material metrics, and materials synthesis and processing. The resultant knowledge supports sharable physics-based models using robust, experimentally-validated multi-scale modeling and simulation for performance prediction and design. Such models will enable the realization and optimization of devices that survive and operate in extreme conditions. Exascale (10^{18} floating point operations per second) computing capabilities, coupled with ARL's state-of-the-art computational and experimental facilities, play a key role in enabling the sharable physics-based modeling capability.

The foundation of the ARL enterprise for multiscale research of materials includes five core program elements to realize a materials-by-design capability, i.e. a modeling and simulation capability that is validated experimentally in time and space to *a priori* design new or improved materials that are uniquely characterized, grown, and processed. These core elements cut across all technical disciplines and are necessary to model, characterize, interrogate, define and synthesize materials. They are:

- *Modeling and Simulation*: Develop computational approaches to predict materials response at relevant length and time scales
- *Bridging the Scales*: Develop physical and mathematical constructs necessary to bridge relevant length and time scales
- *Advanced Experimentation and Validation*: Develop experimental methods to interrogate and characterize the in-situ materials response to extreme dynamic or electromagnetic environments at critical length and time scales for the purposes of discovery and model validation
- *Materials Characteristics and Properties at Multiple Scales*: Establish comprehensive quantitative measures for materials characteristics and properties across critical length and time scales, and develop the parameters in which they may be used to enable further discovery and validation
- *Synthesis and Processing*: Incorporate research discoveries to enable the synthesis and processing of novel materials with critical material characteristics and resulting properties

Without an understanding of the physical processes and properties that govern the interaction of materials from the atomic scale through the device scale, significant time can be wasted in developing new devices and sensors. EMRM is addressing this need for understanding across multiple length and time scales. Since its inception, the EMRM has successfully brought together government and academia to further its stated goals.

2.1. Research in HgCdTe short-wave infrared detectors

Under the EMRM, ARL has collaborated with Boston University (BU), in the area of multiscale modeling of photon detectors.[4] Because of the relationship developed between ARL and BU through the EMRM, ARL has been increasing its modeling efforts in the more focused area of infrared detection using HgCdTe devices.[5-6] Some of this work has focused on numerical modeling of defects related currents in P+-on-n HgCdTe detectors in order to engineer the electric field in a device. The intent here is to understand how to suppress the dark current, which, thereby, reduces the overall noise in an IR detector. The HgCdTe material model used in the numerical simulations discussed below was based on both semi-empirical expressions and atomistic material simulations. For the example, the overlap integral (frequently used as a fitting parameter in the community) used to calculate the Auger recombination rate was previously calculated by Wen *et al.*[7] from first principles using a Green's function formalism. Following this multi-scale approach allows device level simulations to be performed with a minimal set of fitting parameters. The only fitting parameters used are those relating to defects and, as such, are material specific.

Schuster *et al.*, using the input from the lower scale, performed physics-based numerical device modeling of P^+-on-n HgCdTe infrared detectors, designed for operation in the extended short-wave infrared (eSWIR) spectral band, to analyze the performance and characteristics of experimental device data.[5-6] The detectors consisted of a narrow-gap *n*-type absorber layer (AL) followed by a wide-gap *p*-type cap layer (CL), see Figure 1. The analysis revealed the presence of a large generation-recombination (G-R) dark current due to defects. Numerical simulations were then performed that identified heterojunction devices as a means to suppress the G-R dark current in such devices without significantly impacting the quantum efficiency (QE) at the operating bias V = -0.100V.

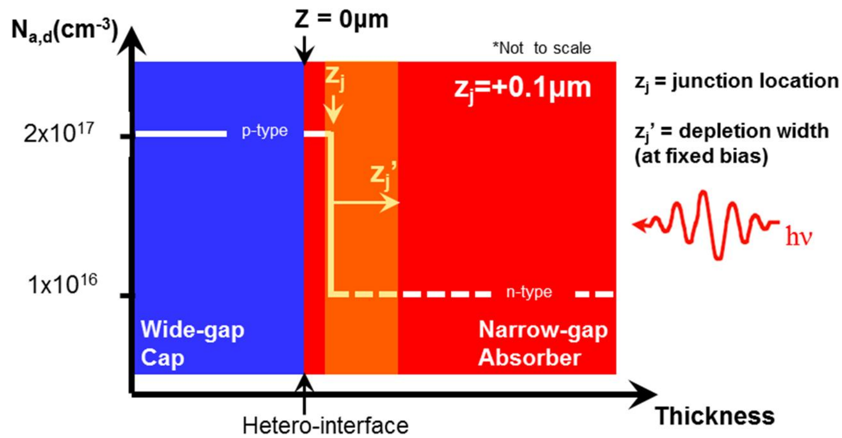

Figure 1. Schematic representation of a single planar P^+-on-n HgCdTe pixel, where red and blue represent the narrow- and wide-gap layers, respectively. Doping concentrations are given by the y-axis, the voltage dependent depletion region is the light shaded area, z_j and z_j'(V) are the implant depth and voltage dependent depletion region penetration into the AL, respectively (relative to the hetero-interface).

In the subsequent analysis, the dark current and QE are numerically determined for various junction depths. Heterojunctions cannot be modeled analytically and, as such, a numerical model is required. For convention the depth of the junction (measured from the AL/CL interface) is given by z_j, see Figure 1. A value of $z_j = 0.0\ \mu m$ indicates that the *p*-type region terminates at the AL/CL interface, $z_j > 0.0\ \mu m$ indicates that the *p*-type region extends into the narrow-gap AL (homojunction) and $z_j < 0.0\ \mu m$ indicates that the *p*-type region resides solely in the CL (heterojunction). Figure 2 presents the dark current (left y -axis) and QE (right y -axis) *versus* z_j at the operating bias V = −0.100 V. For $z_j \geq +0.05\ \mu m$, G-R contributes significantly to the dark current since the majority of the depletion region resides in the narrow-gap AL. However, as $z_j \rightarrow -0.10\ \mu m$, the depletion region resides progressively in the wide-gap CL, eliminating the G-R current. Once the junction is shifted sufficiently into the wide-gap CL, the dark current remains at the diffusion limit until it begins to progressively decrease near $z_j \sim -0.25\ \mu m$. At $z_j < -0.25\ \mu m$, the depletion region does not penetrate sufficiently into the AL (at this bias), which prevents the collection of thermally and optically generated carriers via diffusion. Consequently, the same suppression is seen in the QE, since the diffusion dark current and photocurrent are both mutually dependent diffusion processes. However, even at $z_j \sim -0.25\ \mu m$, QE≈ 90%. Most importantly, the G-R current turns off before the diffusion current does. Thus, there is an optimal regime where the dark current is diffusion limited, without significantly reducing the QE. This optimum resides approximately within $-0.25\ \mu m \leq z_j \leq -0.05\ \mu m$. Numerical modeling studies allowed the parameter space to be rigorously mapped, while avoiding approximations necessary in analytical modeling, to achieve optimal heterojunction device performance by simultaneously optimizing the mutually dependent parameters of dark current and QE. It was demonstrated that an ideal optimization window for these two parameters exists, which cannot be individually assessed to achieve optimal device performance.[5-6]

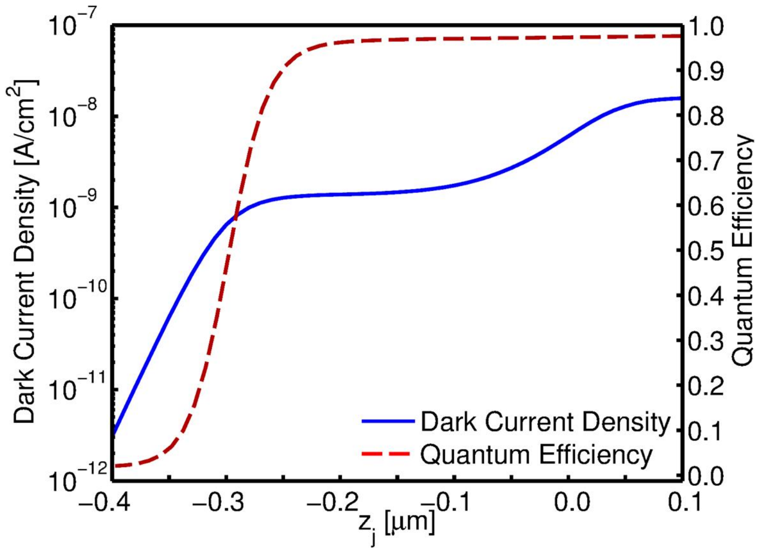

Figure 2. Simulated dark current (left y-axis) and QE (right y-axis) *versus* z_j at the operating bias V = −0.100V. The simulation conditions are T = 200 K, λ = 2.0 µm, and Φ = 1×10^{12} ph/cm^2-s.

3. ARL OPEN CAMPUS CENTERS

ARL's Open Campus initiative is meant to build a new science and technology system that encourages revolutionary advances in fundamental research for US Army applications through extensive collaboration. ARL's Open Campus business model links Army S&T and the global research community through cooperation. Open Campus allows partners in industry and academia to gain the Army's perspective on S&T priorities and to utilize Army expertise, facilities, and capabilities to increase the efficiency of technology transition.[8]

Under Open Campus, opportunities for collaboration begin with mutual interest in research specific to Army needs; investments are made "in-kind," since no funds are exchanged. Open Campus partners can work directly with ARL researchers and share ARL's specialized research facilities. 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.[8] The goal of Open Campus is to foster cutting-edge, Army-relevant fundamental research in a collaborative environment for the benefit of all partners.

Two Open Campus Centers are operating at ARL's Adelphi Laboratory Center. These are the Center for Research in Extreme Batteries (CREB) and the Specialty Electronics Center (SEC). Both of these centers endeavor to bring together academia, industry, and government to focus their respective scientific strengths on innovative research that benefits the members of each center. CREB's goal is to research advanced battery materials and technologies with a focus on extreme performance, environments and properties. The focus of the SEC is on providing access to state-of-the-art research fabrication processes and technologies to obtain valuable, Army relevant, research products by leveraging expertise and high cost semiconductor growth, processing and characterization equipment at the partner facilities. Both the CREB and the SEC function with "in-kind" contributions, the partners each leverage their own research budgets to work collaboratively toward mutual goals set forth by steering committees made up of representatives from the partner organizations. Both centers have attracted interest and funding from other government programs.

4. OPEN CAMPUS CENTER FOR SEMICONDUCTOR MATERIALS MODELING

The goal of the Center is to foster and accelerate collaborative research in the modeling and performance of advanced semiconductor materials and devices. Specific goals seek to improve current materials and devices, and develop and discover new semiconductor materials for sensors, nano-electronics and photonics; transforming new materials into practical devices and sensors (with complete understanding through advanced modeling). The scope of the Center encompasses fundamental research up to and including manufacturing processes.

Key attributes of the Center include integrated 3D multiscale semiconductor modeling (from atoms to sensors); access to unique facilities (e.g. the High Performance Computing Center, the Multi-scale Multi-disciplinary Modeling Cooperative Research Alliance, and the ARL Cleanroom); 3D device models that are anchored to real world device specifications and performance; access to unique research, prototyping and manufacturing facilities; access to unique research solutions for DoD and other applications; access to experienced materials and device engineers and scientists; the ability to tailor intellectual property and compartmentalize as needed; exposure to new ideas and collaborators; the ability to effectively bring together multiple disciplines to engage in collaborative projects; and the ability to formulate joint proposals to seek external funding and technology transition opportunities. All of these attributes are leveraged from the combined capabilities of the partner organizations (government, academia, and industry) for the benefit of all.

The envisioned method of operation of the Center is depicted graphically in Figure 3. In the figure, each of the areas in the path is targeted in order to leverage the strengths of the partners in the Center to increase the overall understanding of the various scales of semiconductor materials. As might be expected, the modeling portion is to increase the fundamental understanding of aspects of semiconductor materials, e.g. modeling the electrical interaction between defects in a material. The modeling feeds into the growth portion to generate examples of the modeled materials to validate the theoretical models in the next step. At this point in the cycle, should the validation fail, the cycle begins anew at the modeling phase to fundamentally understand the reasons behind the failure. Successful validation leads to the characterization phase, where the material's properties are understood within the device environment. This then feeds into modeling for the next scale, and to devices, and then the process repeats. ARL brings to the Center demonstrated capability in materials modeling, growth, and validation. Since potential partners may not have all of these capabilities, complementary projects will be established based upon mutual reliance. Throughout the cycle, other partners in the Center will contribute when the portion of the cycle overlaps their strengths, e.g. novel processing methods and associated validation/characterization may be better suited to industrial partners.

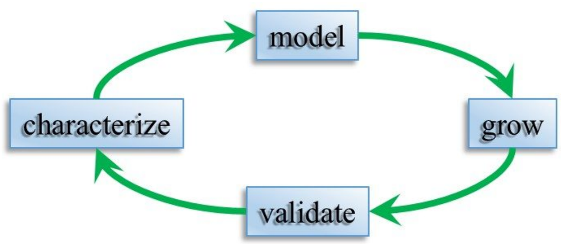

Figure 3. Depiction of the vision for the Center for Semiconductor Materials Modeling.

Participation is open to national and defense labs, universities, and industry with an intended goal of leveraging all relevant capabilities across partners. As depicted in Figure 4, true partnerships will be established with industry and academia through Cooperative Research and Development Agreements (CRADAs) and through Memorandums of Agreement (MOAs) with government agencies. These partnerships serve to further the joint goals of all parties while protecting the intellectual property of the parties. A Steering Committee will be formed with representatives from each Center partner. The Steering Committee oversees the prioritization of projects, availability and allocation of resources, and will continuously evaluate the Center's progress. It is understood that questions and concerns regarding the proposed operation of the Center will arise. These will be mutually resolved by partner organizations as the development of the Center progresses.

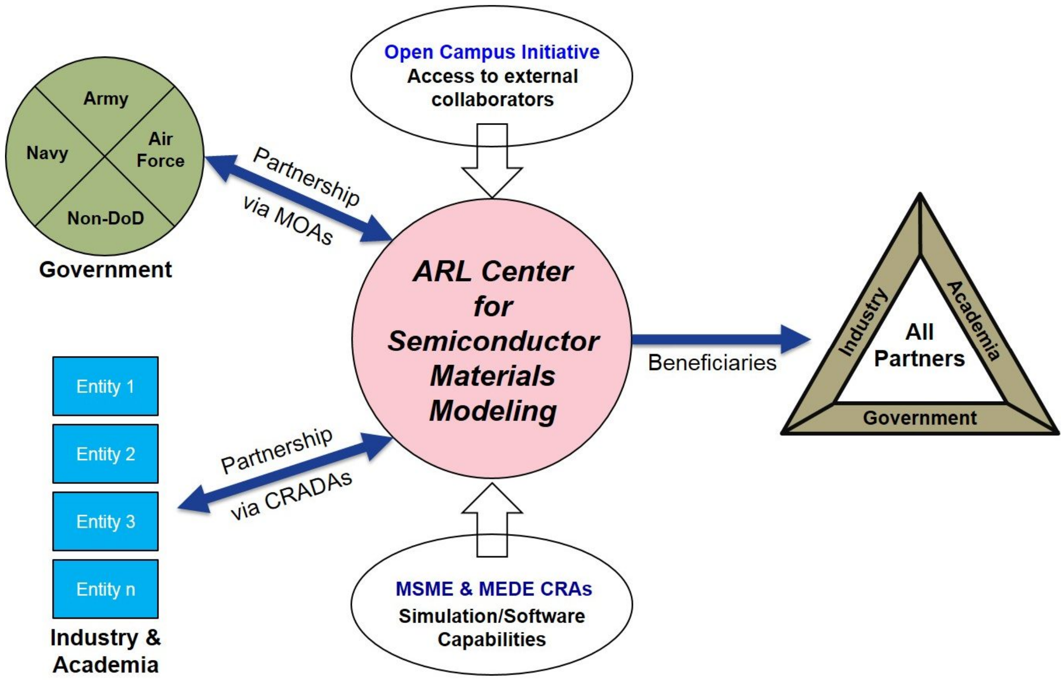

Figure 4. The model for the proposed Center.

The initial focus is on IR and wide bandgap semiconductor materials and devices to provide superior capability for Army applications. The intent is to build upon the ongoing research at ARL and Boston University under the auspices of the EMRM. IR sensor materials are becoming more and more complex, especially with band gap engineering. This has led to development of more sophisticated simulation tools that make it possible to gain insight into new phenomena and to enhance device functionalities and performance. A comprehensive hierarchical multi-scale and multi-physics numerical simulation approach is being developed that consists of a set of modeling tools that extend from fundamental physics-based microscopic analyses to macroscopic engineering based device models.[4] These simulation tools are essential to probing future directions for materials and device development.

The key components to this methodology are a series of first principle numerical modeling techniques, which are used to compute the material properties and device performance. Bellotti[4] divides these into three broad categories:

1. *Atomistic material simulations* – to determine the basic materials properties, such as band structure, effective masses, etc.
2. *Material transport, optical and thermal properties* – to assess the transport and optical properties, using full band Monte Carlo models.
3. *Physical device simulation* – to get device performance parameters, using both commercial and ad hoc simulation codes. Material parameters obtained from fundamental approach are used as inputs.

Figure 5 depicts the progression from the atomic scale to the device scale to the sub-system scale. Each step in the figure has its own modeling challenges associated with the physical processes that govern the behavior. While the progression in figure 5 shows a process for HgCdTe based IR sensors, the Center will expand to other semiconductor materials for sensors, emitters, nano-electronics and photonics applications. For instance, the Center will incorporate ARL's many body theory for photon absorption and luminescence from a III-Nitride quantum well, based on a Greens' function formalism, to advance the understanding of carrier capture and thermal emission from quantum wells, which is needed for enhanced modeling of vertical transport across layers in III-Nitride emitter and detector structures.[9]

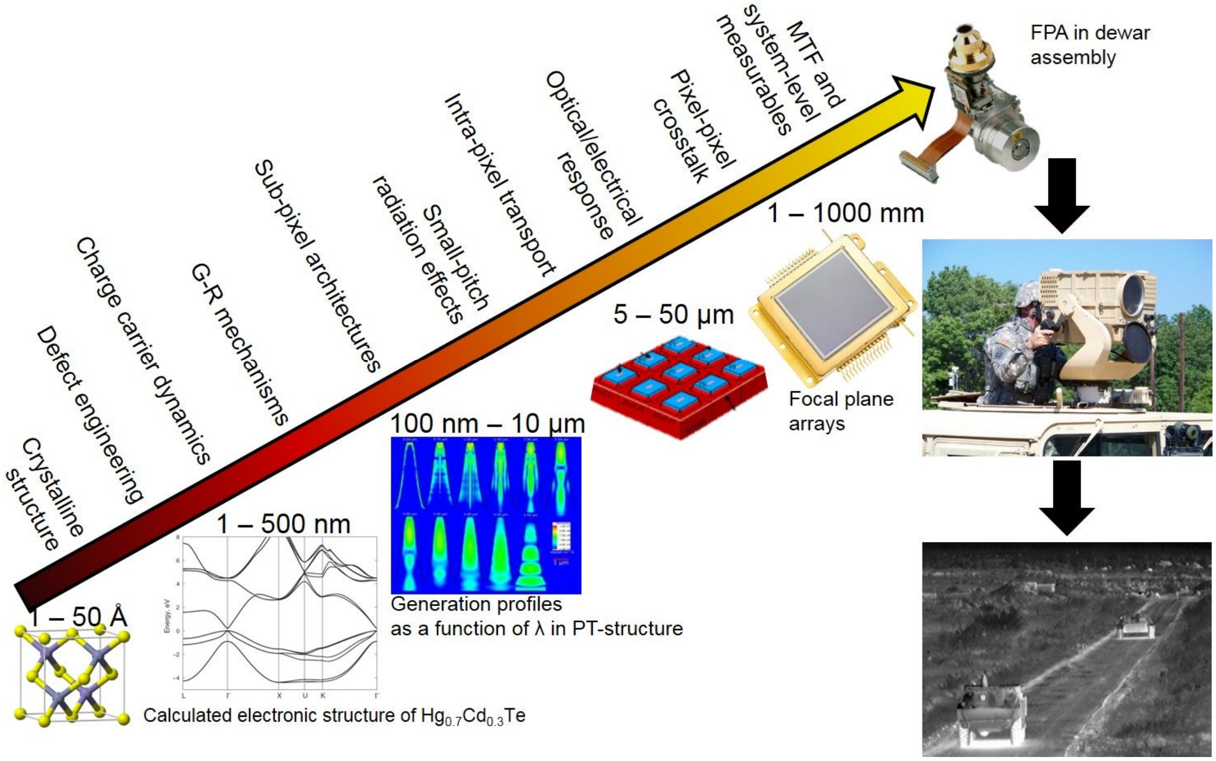

Figure 5. Graphical representation of various scales, from the atomic/crystalline to the sub-system, where modeling can assist in fundamental understanding.

5. CONCLUSION

As the Army progresses in its need for the most capable, most efficient devices built from semiconductor materials, the need for fundamental research in all aspects of the manufacturing process, as a device moves from concept to practice, will increase in order to continuously improve capabilities. Because many of the semiconductor technologies of Army relevance are niche items, there is little drive for industry to expend valuable resources in modeling to arrive at fundamental understanding of any given technology. ARL's proposed Center for Semiconductor Materials Modeling has been devised to address this problem by bringing together government, academia, and industry in a collaborative fashion to continuously push semiconductor research forward so that the ultimate customer, the Soldier, always has the best possible equipment to accomplish the mission.

To move forward toward an establishing a Center, the concept needs to be solidified through critical discussions with potential partners. This will then lead to the steps required to launch the Center. ARL is strategically committed to the formation of the Center and is actively campaigning for its successful initiation in 2016.

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