Center for Semiconductor Modeling of Materials and Devices

Dr. Meredith L. Reed
ARL, Sensors & Electron Devices Directorate
Vision
The Nation’s Premier Laboratory for Land Forces.

Mission
DISCOVER, INNOVATE, and TRANSITION Science and Technology to ensure dominant strategic land power

Making today’s Army and the next Army obsolete
S&T in RDECOM

LCMCs

RDEC Matrixed Engineers to PEO / PMs

RDECs

ARL

Support to Warfighter

Engineering & Production

Advanced Development

Innovation

Discovery

Face-Gear Technology for Block III Apache

XM25 Counter Defilade Target Engagement System

MRAP Armor

MEMS TBI Sensor

Translational Neuroscience

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Human Sciences – e.g. performance enhancement, man-machine integration.

Information Sciences – Information generation, collection, assurance, distribution, and exploitation.

Sciences for Lethality & Protection – weapon & protection systems, Warfighter injury mechanisms...

Sciences for Maneuver – highly adaptive platforms in complex environments

Computational Sciences – computer hardware, high efficiency alg., & mathem. models


Assessment and Analysis: Assess development & application of analytical tools and assess the military utility of combat systems.

Extramural Basic Research
• Inspired by Thomas Edison’s vision of “a great research laboratory” maintained by Government; NRL created in 1923

• In 1945, Bush’s *Science-the Endless Frontier* became model for scientific pursuits

“There are certain kinds of research - such as research on the improvement of existing weapons - which can best be done within the military establishment. However, the job of long-range research involving application of the newest scientific discoveries to military needs should be the responsibility of those civilian scientists in the universities and in industry who are best trained to discharge it thoroughly and successfully. It is essential that both kinds of research go forward and that there be the closest liaison between the two groups.”


Current Defense Laboratory Model

Gates & High Walls provide 20th century security, but are barriers to 21st century innovation

Defense laboratories relatively unchanged since inception!
Responding to the National Security Challenges of the 21st Century

“We will need new technology over the next 10 years to make a leaner and more capable Army.”

GEN Raymond T. Odierno
38th Chief of Staff, Army

Open Campus Website: http://www.arl.army.mil/opencampus/
Aqueous Lithium Ion Batteries

- Collaboration with the University of Maryland through the Center for Research in Extreme Batteries
- Exploring “Water-in-salt” electrolytes to dramatically increase the safety of and maintain the properties of commercial Li-ion batteries.
- Successfully created a completely non-flammable Li-ion battery with performance approaching that of commercial Li-ion batteries.

ARL POC: Kang Xu (Materials Research)

Novel Electronic Devices to Measure Biological Processes

- Collaboration (recent start) with Lehigh University’s Prof. Cheng, who is on sabbatical at ARL
- Investigating methods to measure and model fermentation processes by real-time monitoring of cell-membrane potentials
- Co-developing electronic devices in ARL cleanroom

ARL POC: Chris Sund (Materials Research)
Rate-Activated Tether for Reduction in Ground Impact-Induced TBI

• Collaboration with NFL/Under Armour/GE/ARL
• Concept: Use tether to reduce head velocity during backward falls, and severity of head-to-ground impact
• Rate-activated tether provides over 100X more force during high speed extension, compared to low speed extension

ARL POC: Eric Wetzel (Materials Research)

Information Exploitation Research

• Research to develop analytical solutions to manage uncertainty, speed contextualization, and assist reasoning across multiple sources of information to promote accurate situational awareness.
• ARL and LM(ATL) will endeavor to exploit open-source information, characterize the value of information from an analyst’s perspective, and research advance assisted-reasoning techniques.
• Predictive Analytics
• Characterization of Information
• Exploitation of Open Source / Social Media
• Army Intelligence for Megacities

ARL POC: Tim Hanratty (Information Sciences) / Kevin Barry LM(ATL)
Collaborative Mechanisms

- Cooperative Research and Development Agreements (CRADAs)
- Patent License Agreements
- Educational Partnerships
- Partnership Intermediary Agreements

ARL West

- Local hub for west coast university interactions & recruitment
- Leverage ongoing research at ICT & USC Information Sciences Institute
- ARL-distinct facilities are available at the USC Institute for Collaborative Technology (ICT) UARC
- Excellent potential for increased innovation through closer collaboration with USC & ICT research staff

- Over 390 People Into and Out of Laboratory Under Open Campus so Far
- 91 distinct Collaborators
- 140+ in Staffing
- Over $19M Leveraged from Partners

Active CRADA Projects
Projects Being Negotiated

FY 16
FY 15
FY 14
FY 13
FY 12
FY 11
FY 10

0 50 100 150 200 250 300 350

Mountain View/Palo Alto
Santa Barbara
Playa Vista

The Nation’s Premier Laboratory for Land Forces
Establish a Center for Semiconductor Materials and Device Modeling that brings together government, academia, and industry in a collaborative fashion to continuously push semiconductor research forward for the mutual benefit of all partners.

- Start with HgCdTe
- Expand into other IR materials
- Broaden scope to other material systems

Every Partner is Value Added to The Center
• Timely technology transition with minimal risk requires fundamental understanding of materials synthesis, device operation and design controllable parameters.

• Many of the semiconductor technologies of DoD relevance are niche items; there is little drive for industry alone to expend valuable resources in fundamental understanding. The Government has to take the lead in getting it done.

• 3D numerical-modeling basic-research activities are scattered and insular; not effectively leveraging the combined capabilities of Government, Academia, and Industry. Problems are diverse/complicated, and require multi-disciplined approach.

• As a result technology transition to production is often low yielding, expensive, delayed, and carries operational risk.
Key Attributes of The Center

- Broad Knowledge Base in Semiconductor Modeling
- Combined Modeling, Materials and Device Expertise and Ability
- Computational Resources
  - Pooling of computational tools and resources, (i.e. DoD HPC)
  - Streamlined access to DoD HPC – hours available to ARL collaborators
  - Modeling software: Synopsis, DFT, ANSYS, …
- Continuity
- Extension of the bench
  - Growth, clean room, characterization, fabrication and testing

Leveraging combined capabilities of gov’t, academia, & industry in a collaborative fashion will accelerate semiconductor research to the benefit of all partners
Benefits to DoD
• Procurement and deployment within budget, on time and with minimal risk
• Giving the Soldier the most capable, efficient and reliable devices in the shortest time

Benefits to Industry
• Knowledge-based timely technology development and transition to production
• Increased product yields and lower cost
• Access to unique research solutions
• Expanded market opportunities

Benefits to Academia
• Advancing the state-of-the-art in modeling and materials sciences
• Training personnel in areas with employment opportunities
• Exposure to new ideas and collaborators
• Be aware and contribute to important DoD needs

Creating a National Resource for Atoms-to-Systems Modeling
**Mission**

Develop capability to manipulate matter at any scale, macro to atomic, to create the desired set of material properties and performance.

Program started in 2012

**Three Material Classes**

- Protection Materials
- Electronic Materials
- Energetic Materials

Enterprise Cross-cutting efforts support theories, methods & implementations critical across materials

**Two Collaborative Research Agreements**

**Multi-Scale Modeling of Electronic Materials (MSME)**
- University of Utah and Boston University are the Lead Research Institutions

**Materials in Extreme Dynamic Environment**
- Johns Hopkins is the Lead Research Institution
WHAT IS IT?

Portion of the Enterprise that is devoted to experimental and computational science to design Electronic materials

WHAT DOES IT OFFER?

Revolutionary materials advancements through a multiscale approach for new sensors and electronics for enhanced battlespace effects and efficient power & energy devices

RESEARCH APPROACH:

- Focus on three areas:
  - Electro chemistry
  - Hybrid Photonics
  - Heterogeneous Electronics

- Develop validated multiscale models for:
  - transport, interfaces & defects within semiconductor & energy conversion devices
  - growth, processing, and synthesis of heterogeneous materials

- Use uncertainty-quantified models and large scale computing to predict reliable material and eventually device properties.

Materials by design across relevant scales for efficient, low cost, light weight sensors, and power and energy devices for the Soldier
Materials and Modeling Challenges

Transport:
- At/across interfaces
- Electron or photon transport
- Energy transport

Defects:
- Defects, surfaces or interfaces
- Strain
- Impurities, Vacancies, Interstitials
- Point Defects
- Compositional inhomogeneities

Bridging scales:
- Coarse graining
- Adaptive mesh refinement

- Verification and Validation/Uncertainty Quantification
- Computing multiscale solutions in parallel at large computing scales

ARL resources for realizing validated modeling at and across relevant scales

- DoD HPC
- Modeling: transport, hierarchical modeling simulation, DFT, dislocation dynamics, Green’s function formalism (radiative/nonradiative recombination), etc...
- Growth: II-IV (MBE), III-Nitrides (MBE/MOCVD), III-V’s (MBE)
- Characterization: XRD, AFM, SEM, PL, TRPL, pump probe techniques, ultrafast physics based studies, EL, detector testing, CV, pulsed measurements, etc
- Clean Room: fabrication, mask design, processing
Models can be used stand-alone or to bridge scales. Parameters extracted at each level become inputs for next level.

**Material Modeling**

- Properties
- Carrier Recombination
- Transport Phenomena

**Device Modeling**

- Geometrical effects
- $J(V)$, SR, QE, MTF
- Crosstalk
- Array MTF

**System Modeling**

- Sensitivity
- Dynamic Range
- Resolution (MTF from detector/lenses, etc.)

The Center will develop new and leverage existing models at every scale. Validate performance through growth, processing, and characterization.
Consist of Academia, Industry and OGAs

Multiparty CRADA (Cooperative Research and Development Agreement)
- Between ARL and Academic and Industrial partners within the center
- Define rules for IP and participation within the center

Memorandum of Agreement (MOA)
- Between ARL and other government agencies (OGA)
- Define rules for IP and participation within the center

The Center activities will consist of several Research Projects for which outcomes can be shared amongst members

→ Yearly workshop sharing/exchange of ideas and results

Steering Committee will consist of ARL, Industry and Academic members → oversight of establishing center research projects

Advisory Board will provide guidance on overall direction of the center to ensure Army Relevance

Projects will leverage ongoing funded activities within ARL and their organizations

Opportunities will be identified to secure funding via: NSF, MURI’s, OGAs, DARPA and DOE
**Proposed Modeling Center Logistics**

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**SC: Steering Committee with members from gov't, industry, univ**

- Problem that could be solved by modeling brought forward to the SC

- SC helps form and works together with a project team that defines a solution, initiates project, gets funding

- SC helps get the needed resources, including HPC access. Also helps with addressing any IP or data control

- Team/SC approve information made available to wider audience

- Team reviews project with SC periodically and with larger audience at annual workshops

**Advisory Board**

Via interactions at different levels

Team consists of needed experts in modeling, materials growth, detector and FPA fab and test
What’s needed for a research project to be considered a Center activity?

Outcomes From Research Projects

• Advancing the fundamental understanding of defects, interfaces and transport (or other phenomena) for improved materials and devices that can be shared within the center
• Advanced models and algorithms for developing materials and devices that can be shared within the center
• Collaborative publications

➢ Each team will decide what information will be shared with and whom
➢ Must have an outcome that can be shared within the center

If the Multiparty CRADA for the Center DOES NOT ADDRESS all of information/data sharing amongst the team members
➢ team decides on rules that can be added legally to the multiparty agreement
Participants: 78+ participants

- **28% from Industry:**
  - BAE Systems, CEA Leti, DRS, EPIR, FLIR, HRL, IQE, JPL, L-3, Lockheed Martin, Photon Detector Physics LLC, Raytheon, Skinfrared LLC, SOFRADIR, Teledyne Imaging Sensors,

- **10% from academia:**
  - Boston University, ASU, Harvard, Politecnico di Torino, RPI, University of Illinois at Chicago, University of New Mexico

- **62% from Government:**
  - NVESD (9), AFRL (5), NRL (3), NASA (1), MDA (1), and Sandia National Laboratories (1), ARL (27)
Based on what ARL heard AT the workshop, ARL’s identified the following topics as potential activities that could be pursued within the center:

1) MTF (16%) Working through NVSED with RVS
2) SLS and vertical transport (20%)
3) nBn (20%)
4) Surface charges/passivation (16%) CRADA with RVS
5) heterostructures/interfaces, defects and dislocations (16%) CRADA with RVS
6) APDs, (3D full band Monte Carlo modeling) (12%) (In process of creating JWS/CRADA with GE for UV APDs and SPC)

*Percentages represent what we heard back from participants via EMAIL

Some further long term activities that could be pursued:

7) 1/f noise
8) blinkers
Questions
**Example of MSME Hybrid Photonic Materials**

**Achievement:** IR Materials and Detectors: From Atoms to MTF

A material simulation framework to:

- determine the relevant IR material properties.
- Understand how these properties impact the device performance.
- Understand how to go beyond the fundamental material limits.

Patent submitted by BU (Wichman, Bellotti, Pinkie) for

- Dark current mitigation using Diffusion Control Junctions (DCJ).
- 10 X potential reduction in dark current.
- Working with DRS and ARL to implement in FPA.

Ongoing work with BU CRA PhDs now at ARL/NVESD (Dr J. Schuster and Dr B. Pinkie)

- Simulation capabilities/expertise transferred to ARL/NVESD.
- Working with CRA on next generation of IR sensors.

Recent outcomes from the ARL/MSME efforts provide the basis for creating the Semiconductor Modeling Center now!