Multiscale modeling of transport in optical semiconductors

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S&T Campaign: Computational Sciences
Predictive Sciences

Research objective
• We are developing the capability to do multiscale computations of photo-excitation in semiconductors.
• This will assist in designing materials and heterostructures to be used in sensors and communication devices.
• Employs a two-scale, sequential multiscale method based on Semiconductor Maxwell-Bloch Equations (SMBE)
• In SOA multiscale approaches, relaxation-time approximation (RTA) used for microscale.

ARL Facilities and Capabilities
Available to Support Collaborative Research
• Computation using DoD supercomputers
• Development employs hierarchical multiscale framework to allow near-drop-in use of different solution methods at microscale.
• Framework is scalable and parallelized.
• Active collaboration with semiconductor physicists in SEDD and ARL Materials Enterprise CRA.

Challenges
• Relaxation-time approximation limits accuracy and choice of materials addressed.
• More accurate microscale models exist, but currently limited to homogeneous materials due to computational costs.
• More accurate physical models require significant computational cost, so efficient approaches need for use on high-performance computers.

Complementary Capabilities Sought
• Would like to incorporate a variety of microscale models within the multiscale computational framework.
• Have particular interest in direct Brillouin Zone integration methods for carrier-carrier scattering.
• Also investigating Monte Carlo methods.
• Need capability to compute accurate electronic band structures for a variety of semiconductors.
• Computational methods for far-field electromagnetic radiation.