Multidimensional modeling and simulation of optoelectronic devices

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The understanding and design of optoeletronic devices leads to a variety of mathematical problems arising from the *multiphysics* as well as the *multiscale* nature of semiconductor physics. We will highlight present and future challenges in the **multiphysics modeling** such as:

- transport models for carriers in their self-consistent electrical field ([1, 2, 3]),
- energy transport in semiconductors (i.e. heat generation and conduction in high-power lasers [1] or for self-heating effects in organic electronics [6]),
- the coupling of electronical and optical fields (for laser [1, 5] and photovoltaics),
- new interface models for thin-film solar cells (with active low-dimensional structures), and
- the embedding of quantum-mechanical models for nanostructured parts of the devices ([5]).

In this context many **multiscale effects** are crucial for the functionality of the devices, e.g.

- multi-dimensional problems may have large spatial anisotropies, up to 10^{-5} in state of the art silicon sensors (DEPFET) [2],
- geometrically complex heterostructures occur for vertical cavity surface emitting lasers,
- devices based on semiconductor nanostructures have embedded low-dimensional substructures (quantum well structures, quantum dot layers) [5],
- small-scale interface kinetics or quantum-mechanical description of processes like quantum confinement, scattering and optical transitions on microscopic scale required.

Our *3D device simulator* **WIAS-Oskar3** exploits analytic properties of the models to generate *structure-preserving* and efficient algorithms. Starting from entropy-based thermodynamically consistent multiphysics models ([1, 4]) our discretizations preserve positivity, total mass, and entropy-dissipation. Using highly anisotropic Delaunay meshes the solution methods for the resulting linear systems is based on mathematical and structural properties of the multiphysics system. We will discuss results and challenges arising in the following projects:

- Simulation of quantum dot lasers (in physics SFB 787 ”Semiconductor Nanophotonics” [5]),
- 3D transient simulation of charge clouds in silicon sensors (XFEL) [2],
- Modeling and analysis of active material interfaces in solar cells (PVcomB),
- Modeling and 3D simulation of organic electronic devices ([6], with IAPP Dresden).

References

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