Multiscale approaches for the simulation of electronic devices

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Multiscale approaches for the simulation of semiconductor devices are gaining increasing importance. In particular, coupling of continuous media and atomistic models are of high interest for ultra-scaled electronic devices and for nanostructured light emitting and photovoltaic devices. We will present approaches suitable to couple microscopic and semi-classical transport models, with particular focus on coupled atomistic/continuous calculations.

1. Details

Modeling charge and heat transport or optical properties in downscaled devices requires the use of microscopic models including quantum mechanical effects. On the other hand, nanometer sized active device regions addressed by such models are usually embedded in larger environments, which may influence device behavior in non-trivial manner and therefore have to be considered in the overall device simulation. Since microscopic quantum-mechanical models cannot usually be used on the whole device structure for computational reasons, and since the embedding regions are often described by semi-classical models, multi-scale approaches become necessary [1].

In view of application oriented use of multiscale models, we will illustrate how the relevant models can be integrated transparently in a multiscale/multiphysics simulation environment. Different coupling schemes like bridge and overlap methods will be discussed, and the interaction between atomistic and continuous media models will be described [2, 3]. Based on an engineering point of view, an automated top-down approach is followed for the generation of the atomistic structure, which is based on the macroscopic device description. Possible implementation approaches concerning the association between atomistic structure and finite element mesh, and for the interaction between atomistic and continuous models will be shown.

As examples, we present multiscale simulations coupling linear elasticity, valence force field, k·p, empirical tight-binding, drift-diffusion and non-equilibrium Green's functions for the description of transport or optical properties in MOS transistors, quantum well and quantum dot LED structures, and in organic bistable devices.

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References

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