Advanced Numerical Methods for Semiclassical Transport Simulation in Ultra-Narrow Channels

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Introduction

The first commercialization of the FinFET sparked interest in non-planar, ultra-narrow channels among researchers and manufacturers alike. Questions as to what are the design parameters of such a device or whether the existing FinFET process is optimal have arisen. The influence of strain and usage of materials other than silicon are also hotly debated. As a consequence, the interest in advanced modeling and simulation tools, that could help understand the physics of ultra-narrow channels, is rising. But CMOS is not the only application. There are other fields of research that are investigating the benefits of ultra-narrow channels in various applications, such as silicon thermoelectrics, photovoltaics, or nano-electromechanical systems. These too profit from a sound modeling and simulation framework that can help understand effects and guide experimental efforts.

In this work we present our semiclassical modeling and simulation approach for ultra-narrow channels which has been implemented as part of the Vienna Schrödinger-Poisson (VSP) simulation framework [1, 2] over the past few years. Our research has been driven by two goals: maintaining high physical accuracy of the models while producing a computationally efficient and flexible simulation code.

Physical Accuracy

We achieve the first goal by favoring full numerical models over analytical approximations. First, electronic structure of the channels is computed numerically [3, 4]. The basis for this is the $\mathbf{k}{\cdot}\mathbf{p}$ description of a material's bulk band structure, although our methods are compatible with other electronic structure models as well.

Second, numerical computation of scattering between previously computed electronic states is undertaken. Here, we have pioneered the field by extending the theory of surface/interface roughness scattering to non-planar structures [5, 6]. Other processes such as Coulomb scattering are also given a full numerical treatment, which in the case of Coulomb scattering includes not only dopants in the channel but also charges in the surrounding oxides or at interfaces, image charge, and geometry effects.

Third, we drop unnecessary simplifications to the Boltzmann transport equation (BTE). Such simplifications include neglecting band anisotropy [7] in the context of anisotropic scattering processes and ignoring inter-subband coupling. They are commonly found in literature and used in many simulation codes resulting in errors of up to 20%. We show that directly solving for the distribution functions correctly incorporates anisotropy and inter-subband coupling.

The models are generic enough to be applied to a wide range of semiconductor materials by using the appropriate material parameters. The implementation is dimensionality-agnostic and allows meaningful comparison between bulk, thins films, wires, or fins of any geometry as well as cross-calibration of parameters.

Computational Efficiency

The second goal is achieved by the introduction of several algorithmic innovations. Most of the innovations exploit the sparsity of the different sub-problems. The electronic structure problem is sparse due to the spatial discretization of the $\mathbf{k}{\cdot}\mathbf{p}$-Hamiltonian. This sparsity is taken advantage of in the calculation of the eigenstates. Furthermore, only states are computed that have a low enough energy to contribute to transport. No computation time is wasted on high-energy states.

The Boltzmann transport equation (BTE) is sparse due to energy conservation in discrete $\mathbf{k}$-space. This means that each state can scatter only to a small percentage of other states. Consequently, transition rates are only evaluated for between states that satisfy energy conservation resulting in large time and memory savings.

Even with the exploitation of the BTE sparsity, computing the transition rates remains the most time-consuming part of the process. Thus, the rate calculation was optimized using fast, state-of-the-art algorithms.

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