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VSP - A Multi-Purpose Schrödinger-Poisson Solver for TCAD Applications

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INTRODUCTION

Numerous technological innovations, including material and process changes such as high–k gate dielectrics and metal gate electrodes, are investigated to meet the upcoming scaling requirements. Furthermore, novel structures such as ultra-thin body and multiple-gate MOSFETs are expected to be introduced to suppress short-channel effects [1]. To overcome the technological problems, further theoretical and experimental research is needed which requires an extensive use of computer simulation.

CAPABILITIES

We present the Vienna Schrödinger Poisson solver (VSP) which uses a quantum mechanical transport mode for closed as well as open boundary problems. The thereby calculated carrier concentration is used in the Poisson equation in a self consistent manner. The band structure for electrons and holes is given by an arbitrary number of valley sorts, defined by an anisotropic effective mass and a band edge energy. In this way a wide range of materials can be treated. Also, the effects of substrate orientation as well as strain on the band structure is taken into account.

For investigations of MOS inversion layers, a closed boundary solver using a predictor corrector scheme [2] is applied. VSP includes models for interface traps and bulk traps in arbitrarily stacked gate dielectrics. For the estimation of leakage currents, carriers in quasi bound states (QBS) as well as free carriers are considered [3]. Therefore, direct tunneling and trap assisted tunneling are taken properly into account [4]. These calculations are performed in a post processing step since they have a negligible influence on the electrostatics device behavior. In addition, novel device designs like DG-MOS structures can be investigated.

For systems which are dominated by transport phenomena, like resonant tunneling diodes (RTD), an open boundary solver using the non equilibrium Green's function formalism [5] is available. We use an adaptive method to generate a nonuniform mesh for the energy-space. Very narrow resonances are resolved, while the total number of grid points is kept low, thus delivering stable results at reasonable simulation times [6].

Some typical applications are described in the captions of Fig. 1, Fig. 2 and Fig. 3 respectively.

SOFTWARE TECHNIQUES

The software is written in C++ using state-of-the-art software design techniques. Critical numerical calculations are performed with stable and powerful numerical libraries Blas, Lapack, and Arpack. VSP holds a graphical user interface written in Java, as well as a text based interface. Furthermore, VSP has an open software application interface (API) for the use inside third party simulation environments. These features are used to perform tasks like parameter identification and model calibration, e.g for CV-curves and gate stack optimizations [7].

CONCLUSIONS

We developed a fast and efficient multi-purpose quantum mechanical solver with the aim to aid theoretical as well as experimental research on nanoscale electronic devices. Binaries are available for Linux, Windows, IBM AIX, and MacOs on request.

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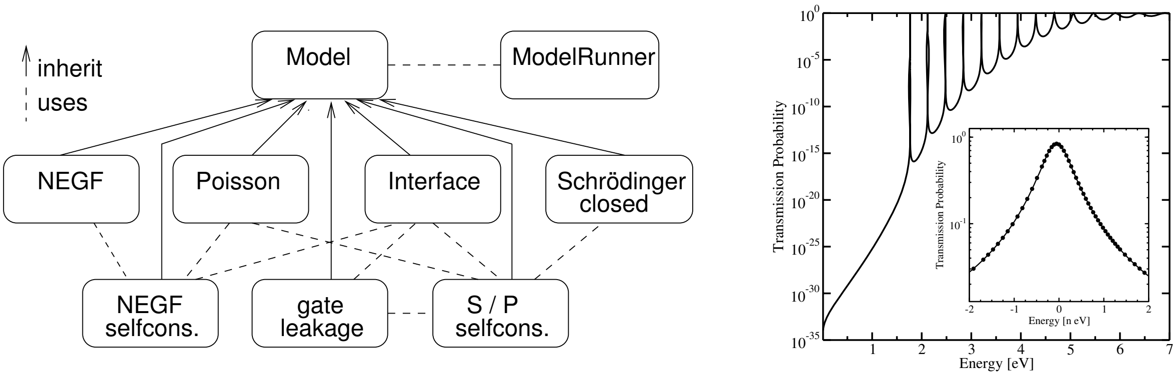

Fig. 1. a) VSP is structured into several models having a common interface. New models can be added easily. b) The transmission probability of carriers through a barrier over an energy range of 7 eV. The inset shows the first resonance in more detail. The width of the first resonance is only a few neV.

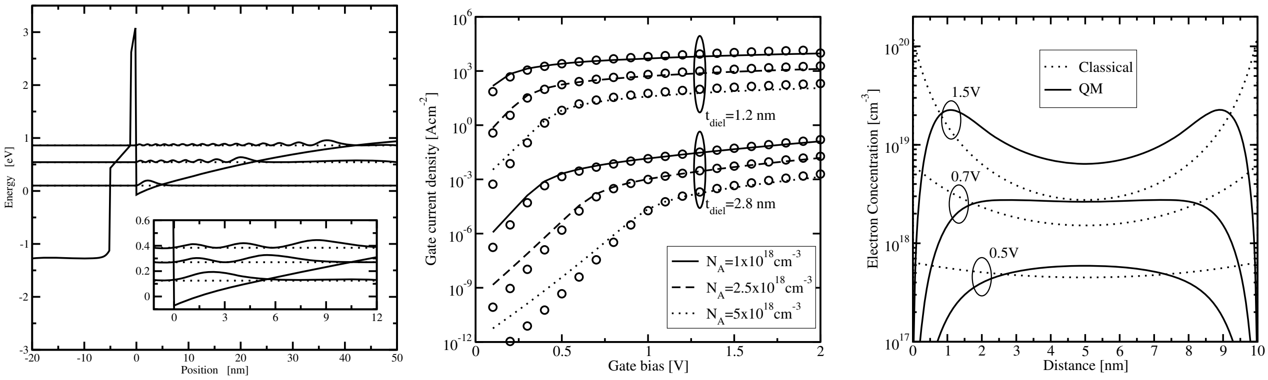

Fig. 2. a) The band edge energy of a MOS-structure with a stacked gate dielectric under inversion conditions. In addition, the wavefunctions and energy levels of some QBS are displayed. b) The estimated leakage current for several MOS-structures based on open–bound and closed–bound eigenvalues which allow much faster calculation [8]. c) A comparison between a quantum-mechanical and a classical calculated electron concentration at different bias voltages for a DG-MOSFET.

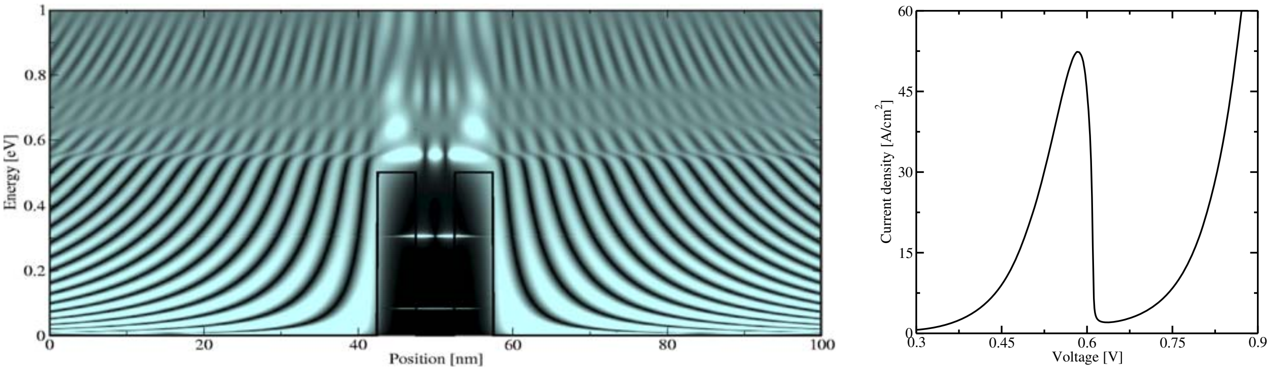

Fig. 3. a) Local density of states of a resonant tunneling diode (RTD) at zero bias. Quantized states are clearly shown in the well. b) IV characteristics of the RTD with open boundary conditions.

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