nextnano^3 – a state-of-the-art simulation tool for 3D quantum nanodevices

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We have developed a simulator for calculating, in a consistent manner, the realistic electronic structure of three-dimensional heterostructure quantum devices under bias and its current density close to equilibrium. The electronic structure is calculated fully quantum mechanically, whereas the current is determined by employing a semiclassical concept of local Fermi levels that are calculated self-consistently.

This code allows one to solve the 8-band-**k.p**-Schrödinger-Poisson equation for arbitrarily shaped 3D heterostructure device geometries, and for any (III-V and Si/Ge) combination of materials and alloys (including ternaries and lattice matched quaternaries, as well as nitrides in the zincblende or wurtzite structure) oriented along any chosen crystallographic growth direction. The method includes band offsets of the minimal and higher band edges, absolute deformation potentials, total elastic strain energy that is minimized for the whole device, the long-range Hartree potential induced by charged impurity distributions, voltage induced charge redistribution, piezo- and pyroelectric charges, as well as surface charges, in a fully self-consistent manner. In addition, magnetic fields can be included. The charge density is calculated for a given applied voltage by assuming the carriers to be in a local equilibrium that is characterized by energy-band dependent local quasi-Fermi levels. These local quasi-Fermi levels are determined by global current conservation, where the current is assumed to be proportional to the density and to the gradient of the quasi-Fermi level (associated with each band) exactly as in the semiclassical limit.

In the calculation of the current, recombination and generation processes can be included. Furthermore, our method automatically includes tunneling via the globally calculated electronic states, and yields optical transition energies and optical matrix elements.

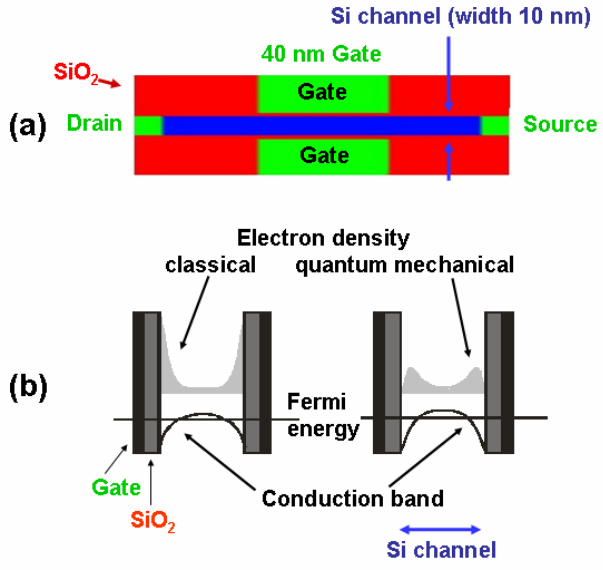

***Fig. 1**:*
(a) Schematic plot of a Double Gate MOSFET
(b) Cut through the 10 nm Si channel: Comparison of classical and quantum mechanical electron density and conduction band edge profile across the Si channel at room temperature. The quantum mechanical simulation gives a smaller current than a classical drift-diffusion calculation (by ~30% for a gate voltage of 0.4 V and drain voltage of 0.2 V).

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For a given nanostructure, the computations start by globally minimizing the total elastic energy using a conjugate gradient method. This yields the local strain tensor which in turn determines the piezoelectric polarization charges, the deformation potentials and band offsets. Subsequently, the multi-band-Schrödinger, Poisson, and current continuity equations are solved iteratively. All equations are discretized according to the finite difference method invoking the box integration scheme. The irregular rectilinear mesh is kept fixed during the calculations.

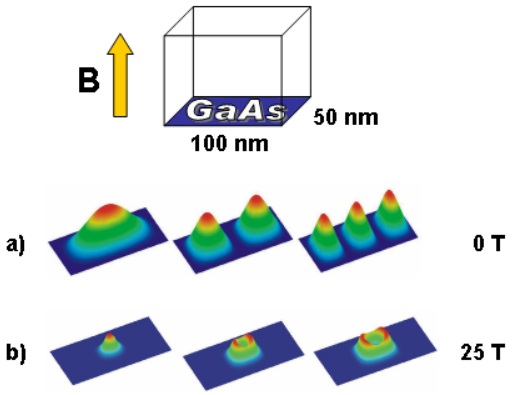

***Fig. 2**:*
(a) Electron density associated with the three lowest eigenstates of a GaAs 2D electron gas confined by high rectangular potential barriers.
(b) Effect of a high magnetic field perpendicular to the GaAs plane on these states. All 3 states shown belong to the lowest Landau level.

The main iteration scheme itself consists of two parts. In the fist part, the wave functions and potential are kept fixed and the quasi-Fermi levels are calculated self-consistently from the current continuity equations, employing a conjugate gradient method and a simple relaxation scheme.

In the second part, the quasi-Fermi levels are kept constant, and the density and the potential are calculated self-consistently from the Schrödinger and Poisson equation. The discrete 8-band Schrödinger equation represents a huge sparse matrix (typically of dimension 10^5 for 3D structures) and is diagonalized using the Jacobi-Davidson method that yields the required inner eigenvalues and eigenfunctions close to the energy gap. To reduce the number of necessary diagonalizations, we employ an efficient predictor-corrector approach to calculate the potential from the nonlinear Poisson equation. In this approach, the wave functions are kept fixed within one iteration and the density is calculated perturbatively from the wave functions of the previous iteration. The nonlinear Poisson equation is solved using a modified Newton method, employing a conjugate gradient method and line minimizations. The code is written in Fortran 90 and consists of some 180.000 lines by now.

For 1D simulations a web based input file generator is available that guides the user through all steps necessary for creating input files. Extensive online documentation as well as several tutorial files are available on the nextnano^3 website at http://www.wsi.tu-muenchen.de/nextnano3 (restricted by login and password). Executables and the source code (tested on Windows, Linux and Unix) are available for download. The material parameters in the database can be adjusted manually. Output files (band structure, densities, wave functions, strain, current, …) can be visualized using standard graphics tools like Origin, AVS, Gsharp or MATLAB. Examples that were treated so far include quantum dots, HEMTs and Double Gate MOSFETs.

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