The 3D nanometer device simulation project next**nano++**

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next**nano**[3] is a versatile software for the simulation of nanometer-scale quantum structures and devices. With this simulator, we can calculate the strain and the associated piezoelectric and pyroelectric charges, the electronic structure in external electric and magnetic fields, optical properties such as excitonic energies and transition matrix elements, or also carrier densities and currents. Almost arbitrary device geometries and material compositions consisting of the zincblende or wurtzite crystal systems are supported [1]. In the following, we will outline some of the basic physical concepts and numerical methods that have been developed for next**nano**[3] or are being developed for the ongoing next**nano**++ project, an international collaborative effort involving many physicists, mathematicians, and programmers. In addition, we will present a few application examples.

The electronic structure is calculated in terms of envelope function in the oneband or multiband k·p-equations. For the latter it is well established that discretization on a grid may result in spurious energy solutions and discontinuities in the wave functions. For this reason, we have developed a new dimension independent box discretization scheme of the multi-band k·p-Hamiltonian that virtually eliminates these problems. Within this method, an artificial diffusion term similar to upwinding schemes is added to the Hamiltonian in order to stabilize the discretization. In addition, the operator ordering employed here avoids singularities in the wave functions.

Another barely recognized problem is that it is numerically extremely difficult to find the correct solution of Schrödinger's equation in the presence of an external magnetic field. Since the magnetic vector potential is spatially unbounded, every naive discretization of the standard minimal coupling Hamiltonian violate the inherent gauge invariance and consequently leads to huge errors in the numerically obtained solutions. We have developed a gauge invariant discretization scheme of the multiband k·p-Hamiltonian that is based on Wilson's formulation of lattice gauge theories. This allows us to calculate the electronic structure and the carrier transport even in the quantum Hall regime.

We have developed and implemented various numerical algorithms to improve the performance and stability of the coupled Poisson-Schrödinger system. For example, the extremal eigenvalues of the k·p-Hamiltonian are calculated using ARPACK in conjunction with a spectral transformation based on Chebyshev polynomials in order to emphasize all relevant eigenstates and to suppress all others. For 8-band calculations, the interior eigenvalues and wave functions are needed. In this case we employ a block variation of the Rayleigh quotient iteration. An efficient and stable block preconditioner, which approximately decouples the electronic components from the spatial variations, is then used to invert the resultant indefinite linear system of equations.

Finally, in order to solve the coupled Poisson-Schrödinger system, we employ an approximate quantum charge density inside of Poisson's equation in order to estimate the dependence of the density on the potential through Schrödinger's equation. Using this estimator the coupling between both equations is much decreased and rapid convergence is achieved. Recently, we have refined this technique further by projecting the Hamiltonian

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into the subspace spanned by all already known eigenvectors, and then diagonalizing this small subspace matrix. With this method only half as much work is needed to obtain the correct solution.

Carrier transport is currently calculated either as ballistic current using the contact block reduction (CBR) method [2] or in terms of an empirical quantum drift-diffusion method. We are currently working on a generalized CBR method that includes scattering within a Büttiker probe model.

In order to achieve a high degree of code reuse we heavily rely on object-orientated programming techniques. An inheritance based class hierarchy combined with the widespread use of C++ templates results into a very efficient and compact implementation without code duplication. All input files use a powerful hierarchical syntax that can easily describe even complicated device geometries. These input files are then parsed using a BISON generated parser module and validated for errors using an approach similar to the one used for validating XML files.

Currently we are using next**nano**^{3} and next**nano**++ extensively to model devices and quantum structures in the Si-SiGe and III-V material systems. Examples for such applications are for instance strained p-channel inversion layers, double gate and wrap-gate MOSFETs (Fig. 1), or also strain-induced T-shaped InAlAs quantum wires, InGaAs/GaAs quantum dot molecules (Fig. 2), and GaN based ISFETs for biosensing applications. CPU time is no longer an issue with next**nano**++, as a self-consistent and fully quantum mechanical 3D electronic structure calculation of a HEMT-type AlGaAs/GaAs device with a total of 4×10^5 grid points requires only about an hour on a standard PC with 2 GB RAM.

The new version next**nano**++ will be made available later this year. In addition to the already extensive documentation tutorials on our website; consulting services are available through Stefan Birner's company next**nano** [1].

[1] See *http://www.wsi.tum.de/nextnano3* for executables and documentation, and *http://www.nextnano.de* for consulting services.

[2] D. Mamaluy, D. Vasileska, M. Sabathil, T. Zibold, and P. Vogl, Phys. Rev. B 71, 245321 (2005), Phys. Rev. B **71**, 245321 (2005).

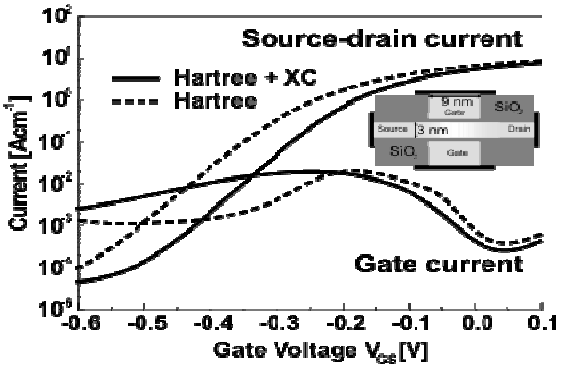

***Fig. 1**: Quantum drift-diffusion currents for the 9nm DGFET shown in the inset. Results from a pure Hartree calculation and one including exchange-correlation are shown.*

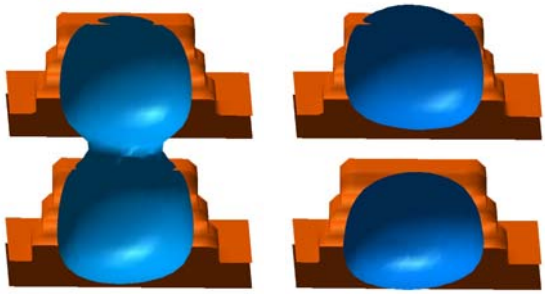

***Fig. 2**: Isosurfaces of bonding and antibonding electron wave functions in two adjacent InGaAs/GaAs quantum dots 6 nm apart from each other.*

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