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OMEN an atomistic and full-band quantum transport simulator for post-CMOS nanodevices

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Abstract—**The technology computer aided design of nanometer-scaled semiconductor devices requires appropriate quantum-mechanical models that capture the atomic granularity of the simulation domain. The recently developed nanodevice simulator OMEN fulfills this condition. It is able to treat two- and three-dimensional transistor structures in a full-band framework using the semi-empirical $sp^3d^5s^*$ tight-binding model. In this formalism each atom of the device is represented by a set of ten orbitals leading to multi-band and open-boundary Schrödinger equations that have to be solved thousands of times. To improve its computational efficiency OMEN has four levels of parallelism that make it run on the largest available supercomputers.**

I. INTRODUCTION

Within the next five to ten years the semiconductor industry will face the greatest challenge in its history. The conventional planar bulk MOSFETs will reach their physical and technical limit and the continuation of Moore's law will depend on novel and original device structures. For example the feasibility of silicon-on-insulator ultra-thin-body (UTB) and multi-gate nanowire (NW) field-effect transistors (FETS) has already been demonstrated by several groups [1], [2], [3].

Modeling such devices requires approaches beyond the classical drift-diffusion and effective mass approximations. The treatment of strong quantization effects as well as the atomic granularity and dimensions of ultra-scaled transistors is demanding state-of-the art physical models. For that purpose we have developed OMEN [4], [6], [7] the first atomistic and full-band quantum transport simulator designed for post-CMOS transistors like UTB and NW FETs that can treat realistically extended and gated devices. A brief summary of its simulation capabilities is presented in this paper.

II. METHOD

OMEN is a two- and three-dimensional Schrödinger-Poisson solver based on the $sp^3d^5s^*$ semi-empirical tight-binding method [8]. This bandstructure model has been chosen for (i) its ability to reproduce the principal bulk characteristics of electrons and holes, (ii) its straight-forward extension to nanostructures, and (iii) its atomic description of the simulation domain. Carrier and current densities are obtained by injecting electrons and holes at different momentum and energies into the device and by solving the resulting system of equations in the Wave Function (WF) or in the Non-equilibrium Green's Function (NEGF) formalism [4]. The treatment of the open-boundary conditions (OBCs) deserves

a special attention since their calculation can generate most of the computational burden if standard techniques such as iterative solvers or generalized eigenvalue problems are used. In OMEN the OBCs are obtained from a shift-and-invert procedure resulting in a normal eigenvalue problem which is at least one order of magnitude faster than the usual approaches [5].

The WF and the NEGF formalisms give the density-of-states (DOS) and the transmission probability (TE) from one contact of the device to the other(s) as function of the injected momentum and energy. The carrier and current densities are calculated by integrating the DOS and TE, respectively and they are self-consistently coupled to the solution of a 2D or 3D Poisson equation. For that purpose a finite-element grid is constructed and the electron and hole charges coming from the tight-binding calculation are represented by delta-functions placed on node positions.

The core operation of OMEN is the calculation of the open-boundary conditions and of the carrier and current densities using either NEGF or WF. This is repeated for each energy, momentum, self-consistent Poisson iteration, and bias point. In a typical 2D UTB simulation N_E=500 to 2000 energy points and N_k=10 to 20 momentum points have to be included for each Poisson iteration and bias point to get accurate results. In other words the Schrödinger equation has to be solved at least 5000 times per bias point. Even if this can be achieved in a couple of seconds the calculation of one single bias point without self-consistency will take hours on a single processor. However, more and more researchers have access to clusters composed of hundreds of processors. To benefit from this resources the computation of the bias points, the energy and momentum integrations, and the spatial decomposition of the simulation domain have been parallelized so that a single simulation can run on a number of processors N_{CPU} comprised between $O(10^3)$ and $O(10^4)$ with an almost perfect speed-up factor of N_{CPU}.

III. RESULTS

Typical device structures that OMEN can handle are shown in Fig. 1 and comprise nanowire field-effect transistors with any cross section shape (square, circular, triangular, hexagonal, $\cdots$), gate architecture (all-around, single, double, or triple), and transport direction ($<$100$>$, $<$110$>$, $<$111$>$, $<$112$>$, $\cdots$) as well as ultra-thin-body FETs with single- or double-gate and any configuration of surface orientation and transport
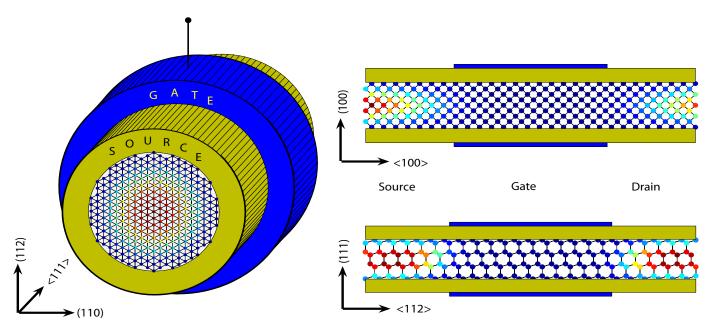
Fig. 1. Schematic view of a circular gate-all-around nanowire (left) and of two double-gate (right) field-effect transistors (FETs) with different transport directions <> and surface orientations (). The nanowire and the ultra-thin-body are surrounded by oxide layers of thickness t_{ox} that isolate them from the metallic gate contacts. The dots represent atoms that are colored according to the carrier distribution. Red atoms depict a high carrier density, blue atoms a low density.

direction. All the channel atoms are represented in the tight-binding formalism. The oxide layers surrounding the channel do not participate to the transport calculation due to a poor parametrization of the material and an insufficient knowledge of their coupling to the semiconductor. The oxide layers are modeled in the Poisson equation as perfect insulators characterized by their relative permittivity ϵ_r and an infinite band gap. Hence, the electrons are confined in the channel and do not penetrate into the oxide as illustrated in Fig. 1.
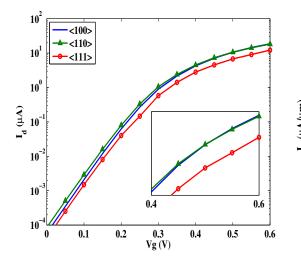
Different semiconductor materials have been parametrized, among them Si, Ge, GaAs, InAs, AlAs, or SiGe. Ternary alloy semiconductors like InGaAs and AlGaAs are treated either as virtual crystals or as atomistically and randomly disordered entities [9]. The parameters are obtained by fitting the band gaps and effective masses of the bulk bandstructure at points of high symmetry. These semi-empirical parameters are assumed unchanged for nanostructures where the surface atoms are passivated.

Current characteristics and internal quantities such as the transmission coefficient, the density-of-states, the carrier density, and the electrostatic potential can be investigated for n- and p-doped transistors. For example in Fig. 2 the logarithmic and ballistic transfer characteristics $I_d - V_{gs}$ of n-doped gate-all-around nanowire transistors with a diameter d=4 nm and a gate length L_g=10 nm are compared for transport along different crystal axis. Similarly in Fig. 3 the ballistic transfer characteristics of n-doped and p-doped double-gate UTB FETS are shown. The six devices have the same dimensions and surface orientation (100), but different transport directions (<100>, <110>, and <111>). Such comparisons are straight-forward in a full-band model, but require lot of

approximations in effective-mass-like approaches.

OMEN offers a good insight into the internal quantities of the simulated devices as illustrated in Fig. 4 and 5. The maximum value of the drain current in Fig. 2 depends on the transport direction. To understand this behavior the corresponding transmission coefficients from the source to the drain contact in Fig. 4 can be investigated. It is observed that the first current channels open for the nanowire with transport along <110>. It is followed by the <100> nanowire that counts two times more channels. The two effects (energy turn-on and number of channels) more or less compensate each other so that the <110> and <100> currents are about the same.

Another important transistor characteristics is its subthreshold swing or the amount of gate voltage change necessary to increase (or decrease) the drain current by one order of magnitude. This information is directly related to the quality of the control one has over the potential barrier induced by the gate contact. Fig. 5 shows the variation of the potential barrier height for two gate voltages and the resulting inversion charges in the channel for a p-doped UTB FET. Ideally a variation of the gate voltage of δV_g would change the barrier height by $q \cdot \delta V_g$ where q is the elementary charge.

The transport in OMEN is not restricted to its ballistic component, but elastic scattering like surface roughness [6] and alloy disorder [9] can be fully taken into account due to the atomic nature of the simulation domain. For a given device configuration one can study the most advantageous transport direction and surface orientation with respect to ON- and OFF-current, subthreshold swing, drain-induced barrier lowering, source-to-drain tunneling, transient time, and sensitivity to surface roughness.
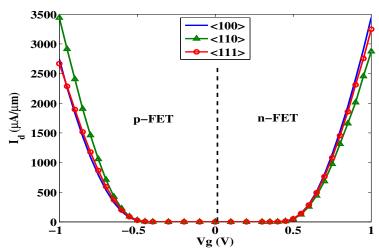
Fig. 2. Transfer characteristics $I_d - V_{gs}$ (V_{ds}=0.6 V) of n-doped Si gate-all-around nanowire FETs (diameter d=4 nm, gate length L_g=10 nm) with transport along the <100>, the <110>, and the <111> crystal axis.

Fig. 3. Transfer characteristics $I_d - V_{gs}$ (V_{ds}=±1.0 V) of n- (right) and p- (left) doped Si double-gate ultra-thin body (DG UTB) FETS (body thickness t_{Si}=4.9 nm, gate length L_g=22 nm) with (110) as surface orientation and transport along the <100>, the <110>, and the <111> crystal axis.
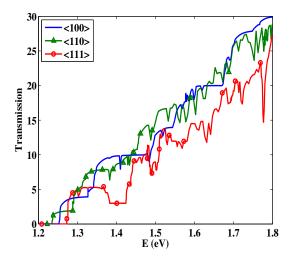

Fig. 4. Transmission coefficient through the same gate-all-around nanowire FETs as in Fig. 2 at $V_{gs}=V_{ds}$=0.6 V. The energy reference E=0.0 eV is the top of the bulk valence band.
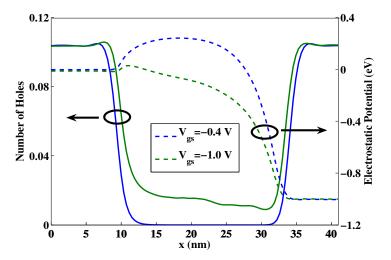

Fig. 5. Number of holes (solid lines) and inverse average electrostatic potential (dashed lines) along the transport direction of the <110>/(110) DG UTB simulated in Fig. 3. Results were obtained at V_{ds}=-1.0 V.

The multi-level parallel implementation of OMEN and the optimization of its numerical algorithm make the simulation of NW with a cross section up to 22 nm^2 and UTB with a body thickness up to 10 nm and a gate length of L_g=40 nm possible. For a realistic UTB structure designed according to the 22 nm technology node specifications an almost ideal scaling of the simulation walltime up to 32768 processors can be demonstrated [10]. In Fig. 6 the walltime measured for the simulation of a circular nanowire FET (green curve with triangle, diameter d=3nm, gate length L_g=15 nm) and a double-gate UTB FET (blue curve with crosses, body thickness t_{body}=4.9 nm, gate length L_g=22 nm) are reported as function of the number of processors used. The dashed line indicates the ideal scaling slope.
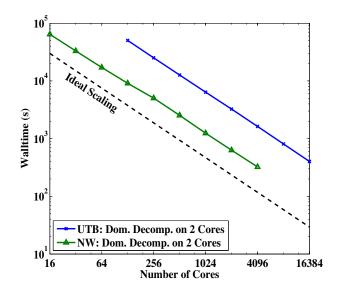
IV. CONCLUSION

At the moment no other full-band and atomistic quantum transport simulator offers such physical capabilities, computational efficiency, and support in developing nanotransistors as OMEN. Gate leakage currents, surface reconfiguration, discrete doping atoms, and dissipative electron-phonon scattering are planned for future extensions.

ACKNOWLEDGMENT

Fig. 6. OMEN scaling performance for the computation of the transfer characteristics $I_d - V_{gs}$ of a UTB (same structure as in Fig. 3, blue curve with crosses) and a circular nanowire (diameter of 3 nm, green curve with triangles) field-effect transistor. The four levels of parallelism of OMEN are turned on for the UTB case (8 bias points, 16 momentum points, about 1400 energy points, and domain decomposition on 2 cores). The nanowire simulation requires three levels of parallelism (16 bias points, no momentum, about 540 energy points, and domain decomposition on 2 processors).

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