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Multimillion Atom Simulations with NEMO 3-D

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Full-Band and Atomistic Simulation of Realistic 40 nm InAs HEMT

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Abstract
A realistic 40 nm InAs high electron mobility transistor is studied using a two-dimensional, full-band, and atomistic Schrödinger-Poisson solver based on the $sp^3d^5s^*$ tight-binding model. Bandstructure non-parabolicity effects, strain, alloy disorder in the InGaAs and InAlAs barriers, as well as band-to-band tunneling in the transistor OFF-state are automatically included through the full-band atomistic model. The source and drain contact extensions are taken into account a posteriori by adding two series resistances to the device channel. The simulated current characteristics are compared to measured data and show a good quantitative agreement.

Introduction
The scaling properties of high electron mobility transistors (HEMTs) with III-V compound semiconductor channels are currently investigated by both industry and academia. The logic performance of InGaAs and InAs based HEMTs with a gate length and a multi-quantum-well channel thickness scaled down to 40 and 10 nm, respectively has been recently reported [1,2]. It is expected that such devices will profit from the very high mobility of InAs, 20,000 cm²/Vs, to exhibit high-speed operation, low-power consumption, and to outperform the conventional Si devices.

The interest in physics-based computer design to develop novel technology such as InAs HEMTs has considerably increased in the last decade. However standard techniques such as drift-diffusion are not adapted to the nanoscale devices shown in Ref. [1] and [2]. In effect they cannot capture the strong confinement of the electrons and the resulting quantization of the energy levels. In order to remedy to this deficiency quantum mechanical treatments within the effective mass approximation have been recently proposed for III-V devices [3]. However, the non-parabolicity of the InAs lowest conduction band is missing so that the electron states cannot be correctly populated. At a higher level full-band simulations have also been attempted, but they are restricted to very small Si structures [4] (channel thickness of 3 nm, total length of less than 30 nm) or they are based on semi-classical one-dimensional approaches [5].

In this paper we present a highly-efficient ballistic, two-dimensional, full-band, atomic, and quantum mechanical simulator [6,7] to study realistic InAs HETMs with InGaAs and InAlAs barriers as proposed in Ref. [2]. The tool is based on the nearest-neighbor $sp^3d^5s^*$ tight-binding model and a Wave Function approach, equivalent to the Non-Equilibrium Green’s Function formalism, but computationally much more efficient in the case of ballistic transport. Its four levels of parallelism and its optimized numerical algorithms allow the simulation of 140 nm long devices with a channel thickness up to 12 nm [8]. This goes much beyond the capabilities of any other full-band atomistic simulator. Furthermore, quantitative agreement with the experimental data of Ref. [2] is obtained.

Approach
The computer-aided investigation of large devices such as the HEMT depicted in Fig. 1 requires the establishment of a three-level hierarchy of the simulation domain, one for the strain relaxation (entire structure), one for Poisson equation (region delimited by the black dashed line), and one for the quantum transport problem (shaded region).

The valence-force-field (VFF) method with a Keating potential is used to relax the atom positions in the channel [9]. Strain is caused by the InAs-InGaAs and InAs-InAlAs lattice mismatch. In effect In$_{0.53}$Ga$_{0.47}$As has a lattice constant $a_0$ of 0.5868 nm (same as InP) so that the thin InAs layer grown on top of it ($a_0=0.60583$ nm) undergoes a biaxial compression. Since strain is a long range effect its calculation extends over a volume of 1,414,400 atoms, starting from the InP substrate while the atomistic transport domain contains 38,556 atoms.

The 2D Poisson equation is solved with the finite element method on a domain that includes the gate contact (Dirichlet) and whose electrical field vanishes at the other boundaries (Neumann). For computational reasons only 20 nm of the lower InAlAs layer are taken into account. Finally, we simulate the atomistic and full-band transport properties of the active region using the approach described in Ref. [6] and [7]. Electrons are injected into the device at different wave vector and energy values and the resulting contributions are summed up to give carrier and current densities. We consider each atom individually so that random alloy disorder is automatically taken into account. The $sp^3d^5s^*$ tight-binding parameters for InAs, GaAs, and AlAs are taken from Ref. [9] and [10]. Spin-orbit coupling and hole transport are neglected, except for the calculation of the band-to-band tunneling OFF-currents.

To model the source and drain extensions of the device we attach two series resistances $R_S$ and $R_D$ to the quantum transport domain as shown in Fig. 1. Hence, the electrons in the channel see an effectively reduced drain-to-source $V_{ids}=V_{ds}-(R_S+R_D)I_d$ and gate-to-source $V_{igs}=V_{gs}-R_SI_d$ voltages as compared to the externally applied $V_{ds}$ and $V_{gs}$.

The variable $I_d$ represents the simulated drain current.

Results
The InAs HEMT shown in Fig. 1 is studied to illustrate the capabilities of our simulator. It is based on the device
The gate length $L_g$ of 40 nm, an insulator thickness $t_{ins}$ of 4 nm, a source and drain injection region of 50 nm, and transport along the $<100>$ crystal axis. The active region is composed of a In$_{0.52}$Al$_{0.48}$As (3 nm) - InAs (5 nm) - In$_{0.53}$Ga$_{0.47}$As (2 nm) multi-quantum-well structure. To account for the penetration of the electrons into the upper In$_{0.52}$Al$_{0.48}$As insulator 2 nm of this layer are included in the quantum mechanical calculation. In the transport direction 140 nm are simulated so that the full-band and atomistic regions becomes a $12 \times 140$ nm$^2$ rectangular. The doping of the structure is realized with a delta-doped layer placed just below the gate contact and whose donor concentration is $N_D=3 \times 10^{12}$ 1/cm$^2$. The value of the source and drain series resistance is set to $R_S=R_D=190 \ \Omega \cdot \mu m$ to correctly reproduce the $dI/dV_{ds}$ current slope at $V_{gs}=0.4 \ \text{V}$.

In Fig. 2 and 3 the lattice constants of the structure along the transport ($x$) and growth ($y$) directions are depicted. The relaxation of the atom positions is calculated either with the VFF method (black line) or assuming a uniform biaxial strain tensor (gray line with circles). As it can be observed in these two figures the uniform biaxial strain tensor is a good approximation along the transport direction, but fails to capture the correct relaxation of the atom positions along the growth direction.
The bandstructure of the multi-quantum-well active region is given in Fig. 4. Due to the compressive biaxial strain the conduction subbands are pushed to higher energy levels. At the same time and for the same reason the valence subbands (not shown here) are pushed down in energy. Hence, under the influence of strain and carrier confinement the effective band gap of the InGaAs - InAs - InGaAs structure is raised to about 0.77 eV, more than twice the bulk value of $E_g=0.37$ eV. Similarly, the effective mass of the lowest conduction subband increases from 0.024-$m_0$ (bulk) to 0.043-$m_0$ due to the finite thickness of the InAs body.

The larger electron effective mass and band gap are advantageous to manage the OFF-current of the device. In effect they induce a quasi suppression of band-to-band tunneling at low $V_{gs}$ ($\leq -0.2$ V) and high $V_{ds}$ (0.5 V). The OFF-current is mainly dominated by gate leakage (not considered here) and small thermionic emission. This is illustrated in Fig. 5 where the simulated thermionic and band-to-band tunneling currents are compared to the measurement of Ref. [2]. However, the maximum carrier velocity is proportional to $1/\sqrt{m^*}$ and therefore suffers from the effective mass increase as the OFF-current. Note that the effective mass value is determined by the confinement of the electrons, and not by strain so that a thinner InAs layer gives a higher conduction band effective mass and a lower mobility limit.

Further comparisons between the experimental data from Ref. [2] and simulation results can be found in Fig. 6 to 8. Some of the most important transistor metrics like ON-current, threshold voltage, subthreshold swing, drain-induced barrier lowering, and transconductance maximum are summarized in Fig. 9. Good quantitative agreement is achieved for the transfer and output characteristics, except at high gate voltages where electron-phonon scattering may still play an important role. In Fig. 8 the slope of the simulated transconductance is
Simulation and atomistic simulation of realistic 40 nm HEMT with quantitative agreement to experimental data. The tool has now been calibrated to study the scaling behavior of multi-quantum-well InAs channel down to 22 nm and below.

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