Atomistic Simulation of Nanoscaled Devices

Group Profile

The Glasgow Device Modelling group is one of the largest specialised semiconductor device modelling groups worldwide with critical mass and expertise encompassing semiconductor, solid state and quantum theory, simulation techniques, numerical algorithms, advanced programming, parallel processing, device operation and design, and system architectures. Members of the group were early pioneers of the theory of ultra-small semiconductor devices [1-3] and developed many of the established tools of quantum transport theory appropriate to high field transport in small structures [4-9] including studies of quantum corrections to device simulation [10-13] and quantum transport in high electric fields [4-9]. In recent years we have led both the commercial players and other major international research groups, in developing a unique 2D finite element Monte Carlo simulator H2F [14-19] which can perform time domain RF analysis of complex shape HEMTs, properly taking into account all device parasitics. We are one of the few groups worldwide with in-house full-band 2D/3D ensemble Monte Carlo simulation capabilities, developed initially for p-type SiGe devices [20, 21]. We were also one of the first groups to recognise the significance of the fluctuation potential in compromising useful quantum coherence in mesoscopic semiconductor devices [22-24]. Now we are recognised as world leaders in the simulation of intrinsic fluctuations in ultra-small MOSFETs introduced by the discreteness of charge and atomicity of matter. In this area we have :

- Developed the first quantum 'atomistic' 3D simulator [25-28] (Figs. 1, 2) which takes into account statistically the effects of discrete random dopants in decanano devices [29, 30];
- Calculated, for the first time, the magnitude of MOSFET intrinsic parameter fluctuations introduced by atomic scale interface roughness and the corresponding local oxide thickness variations in devices with ultra-thin gated oxides [31, 32];
- Performed statistical, gate line edge roughness simulations of 3D MOSFETs [33] for the first time (Fig. 3).
- Evaluated a variety of fluctuation resistant MOSFET architectures [30, 34, 35].

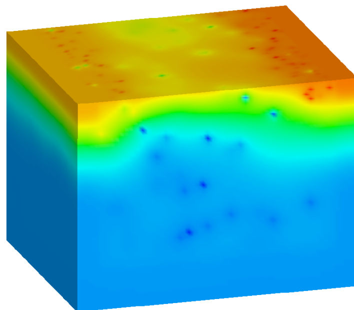

Fig. 1 The potential distribution obtained from the 3D 'atomistic' quantum simulation of a 30×30 nm MOSFET illustrating potential fluctuations in the channel introduced by individual discrete dopants.

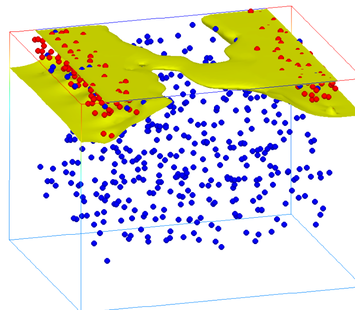

Fig. 2 The corresponding 3D electron concentration distribution. The vertical quantum confinement effect results in a maximum in the electron concentration approx 1nm below the interface. Lateral confinement effects are also visible.

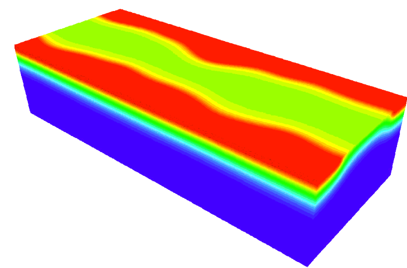

Fig. 3 Potential distribution obtained from the simulation of a 30×100 nm MOSFET which takes into account the line edge roughness (LER) of the of the polysilicon gate. The LER introduces variations in MOSFET parameters from device to device.

Currently the Group facilitates the design of aggressively scaled Pseudomorphic High Electron Mobility (HEMT) transistors with dimensions down to 30nm for the Ultrafast Systems Group at Glasgow and metamorphic HEMTs on 'virtual substrates' for Caswell [36-38]. We provide full simulation support for the UK SiGe HMOS consortium of eight universities with industrial partners Zarlink, Daimler-Chrysler, Infineon and Synopsis, which includes physical simulation and design of a variety of SiGe based MOSFET

architectures [18, 19, 39-42]. We have ongoing collaborations with the IBM T. J. Watson Research Centre, Yorktown Heights; NASA Ames Research Centre, Moffet Field [30]; NASA Jet Propulsion Laboratory (JPL), Pasadena; Intel, Santa Clara [33]; Motorola Analog-Mixed Signal Technology Centre, Tempe; the Naval Research Laboratory, Washington; Arizona State University [43]; Purdue University and Ohio Universities [33, 31] in the area of atomistic and quantum transport simulation.

The group publishes an average of ten papers p.a. in quality international journals, complemented by a larger number of conference papers in the leading device and simulation conferences and gives similar number of invited talks p.a. This includes two papers p.a. in IEEE Transactions on Electron Devices during the last four years [14, 29, 25, 35, 30, 28, 31] and a papers in IEDM [27, 34], SISPAD [28, 32, 33, 40, 43, 44] and ESSDERC [37, 38, 41]. Recent invited talks by group members include presentations at IBM Yorktown Heights, NASA Ames, Intel Santa Clara, ESSDERC, SISPAD, MSM, IWCE and ChiPPS. Members of the group have organised/co-organised several international conferences focussing on ultra-small semiconductor devices including two NATO ASIs on the Physics of Non-Linear Transport in Semiconductors (1979) and the Physics of Granular Electronic Systems (1991), the 7th International Workshop on Computational Electronics (IWCE-2000) in Glasgow, the first Advanced Research Workshop on Quantum Transport in Semiconductors, Maratea (2001) and the Silicon Nanoelectronics Workshop, Honolulu (2002).

We are one of the best equipped modelling groups in the world, hosting an 8 processor Origin 2000 system provided by NASA Ames, a 40 processor IBM pSeries 640 system donated by IBM, sharing access to a 30 processor Sun Enterprise SMP system provided by SHEFC and a new 32 processor Origin 300 system. This is complemented by access to the NASA Information Power Grid through NASA Ames. The group enjoys a beneficial relationship with the largest vendor of commercial process and device simulation software, Synopsis.

Strategic View

The aims of this Platform Grant are to sustain the talent, the expertise, the critical mass and the internationally leading reputation of the Glasgow device modelling group and to enable the development of our next generation of simulation methods and tools, which can meet the challenges facing simulation and design of the decanano-scale semiconductor devices which will be in mass production by the second half of this decade, and the nano-scale devices expected in fifteen years time [45].

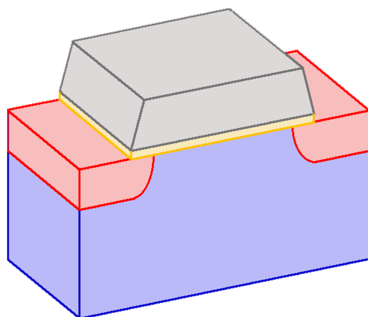

Fig. 4 The current approach to semiconductor device simulation assumes continuous ionised dopant charge and smooth boundaries and interfaces.

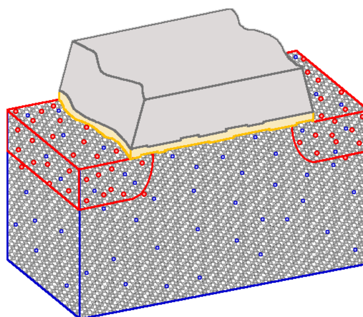

Fig. 5 Sketch of a 22 nm MOSFET expected in mass production in 2008. There are less than 50 Si atoms along channel. Random discrete dopants, atomic scale interface roughness and line edge roughness introduce significant parameter fluctuations.

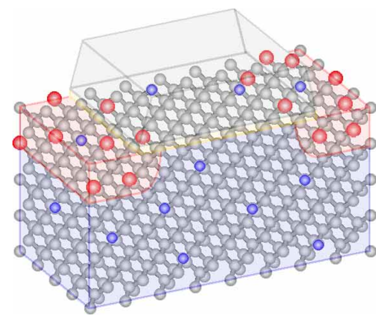

Fig. 6 Sketch of a 4 nm MOSFET expected in mass production in 2023. There are less than 10 Si atoms along the channel. The size of the device becomes smaller than the size of a large molecule.

As seen in Figs. 4, 5 and 6, at nanometer scale the active region of a MOSFET becomes comparable to the size of a large molecule. We aim to develop simulation methods and tools that will bridge the gap between the present continuous classical and quantum semiconductor device simulation approaches and the *ab-initio* methods of quantum chemistry in describing, with progressive accuracy, phenomena related to

- The discreteness of charge and matter at an individual dopant and carrier level;
- Quantum transport at the atomic scale.
- Statistical intrinsic parameter fluctuations associated with random dopants, imperfect interfaces, boundaries and contacts in ultrasmall devices.

Such methods and tools can also be relevant for simulation of molecular and bio-molecular structures and devices for the post-silicon era and we would like to establish a presence in this area.

It is clear that in nano-scale devices with critical dimensions measured in tens or single lattice spacings, the granularity of charge and matter has to be properly accounted for. The simulation paradigm shifts from techniques considering the device as a continuous media and based on the solution of the Boltzmann Transport Equation (BTE) to near first-principles quantum approaches which consider the device as a collection of atoms or ions and calculate the current based on the individual and collective motion of charges. It must be noted that the traditional ensemble Monte Carlo simulation approach does not meet this criteria, being simply a statistical technique for solving the continuous BTE. Although we are the world leaders in the area of statistical 3D atomistic simulation our present atomistic simulator mainly accounts for the electrostatics of individual discrete dopants, rough interfaces and line edge roughness and implements simple quantum corrections based on the Density Gradient algorithm [26, 46]. More complex problems associated with random variation in the impurity and surface limited mobility, interface states and localised tunnelling through a few atomic layers of oxide, noise and plasma coupling between the individual carriers in the channel and the adjacent regions have to be treated at an atomistic level. It is still conceptually unclear how to marry the costly *equilibrium*, *ab-initio,* atomistic simulation techniques [47] used extensively in computational chemistry with transport in nano-scale devices. We wish to explore the possible intermediate levels of complexity including particle-mesh simulation with discrete dopants at the individual electron level [47], progressively introducing corrections based on Quantum Hydrodynamic [48-53], Wigner [6, 7, 9, 54-57], and Green [54] function formalisms. Many-body effects are recognised to be crucial at the high densities associated with nano-scale devices, and it is proposed to extend quantum descriptions of semiconductor transport to this regime, building on our earlier work on few-body quantum transport [58-60], field-dependent screening [8, 61] and single-electronic charging effects [58, 62, 63]. We intend advancing to *non-equilibrium*, first-principle approaches [64] where the quantum description of electron transport might possibly be based on a functional representation of many-body quantum states in terms of currents and densities as generalised "coordinates" [65]. New numerical techniques will be explored which provide significant speed enhancements for carrier-carrier scattering and for quantum evolution.

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