Introduction

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Device miniaturization has been a major trend in microelectronics for almost fifty years, allowing for continuous enhancement of chip performance and functionalities. However, conventional downscaling of Metal-Oxide-Semiconductor (MOS) technologies is gradually replaced by a multiplicity of novel device architectures based on properties of matter at the nanoscale, and even at the molecular scale, but also with the introduction of complex materials in devices, such as high-k oxide stacks, stressor layers, III-V-based channel, etc. . .

In this context, Technology Computer Aided Design (TCAD) has become critical all along the technology development since it makes possible extensive process exploration and provides inputs for material and device optimization. However, TCAD tools are based on semi-empirical models and require calibration before being predictive and therefore operational in an industrial environment. For the last decades, during which the Moore law has basically been achieved by scaling bulk silicon device geometries, this mandatory calibration step was achieved by gathering information and model parameters from the experimental data available from previous technological nodes. This has become a much more critical step due to the increasing complexity of the process, the acceleration of the technology development, and breakthroughs in devices architectures and materials. In certain cases, experimental data are even miss-

ing or incomplete, and a standard calibration procedure of TCAD tools has become incredibly complex.

In order to meet the needs of the MOS industry and to make practical exploitation of alternative devices, a new generation of simulation tools is emerging. The electron device community is currently investigating new integrated simulation approaches accounting for a broad range of physical principles introduced by the reduced dimensionality and the multiphysics nature of the problems to be solved. At these scales, the distinction between material and device modelling is getting increasingly blurred. The electronic and transport properties of the system can sharply depart from those of bulk materials and become dependent on the detailed device geometry. In addition, heat dissipation can also be hampered, with self-heating effects calling for careful thermal management. The increasing research activity in the fields of thermoelectric and photovoltaic devices is also a strong motivation towards the development of multiphysics modeling approaches.

Meanwhile, novel fundamental approaches are gradually used for the investigation of new material: III-V semiconductors on silicon, used as high mobility channels, new materials for the contacts and the oxides, and even more exotic 2D or 1D materials such as silicon nanowires, graphene nanoribbons and carbon nanotubes. First-principles methods have been developed to solve complex and fundamental problems in very small systems. They are now commonly used to calibrate accurately semi-empirical models and even to treat transport problems in nanodevices. It illustrates the fascinating tendency to connect tightly and consistently several models from the atomic level to the device and even circuit levels with an increasing accuracy. It is considered now as a requirement for the credible emergence of nanosciences in the real world of applications.

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This special issue on multiscale and multiphysics modeling contains nineteen papers which overview a broad range of what the prefix “multi” may cover. It illustrates the increasing need for such complex approaches which combines either different levels of the same type of problems that cannot be fully treated using a single method, or different problems that complicatedly interact with each other.

A first set of papers is dedicated to multiphysics simulation, where different coupled phenomena have to be considered simultaneously. Zanuccoli et al. demonstrate the possibility to combine two numerical tools to perform electro-optical simulation in order to investigate critical issues of photovoltaic applications, in particular of solar cell efficiency. The drift-diffusion electron transport is coupled to a solver of Maxwell equations based on the Rigorous Coupled-Wave Analysis (RCWA) method. This approach is applied in-depth investigation of a solar cell based on an array of nanowires. The coupled effects of electrons and phonons are considered in two different approaches for two kinds of problem. Vasileska et al. study the self-heating effects in fully-depleted SOI transistors. Using the Sondheimer’s approach they first calculate the thermal conductivity of silicon thin films including anisotropy effects, in excellent agreement with experiments. This conductivity model is then used in the higher level modeling of self-heating effects in fully-depleted devices that is based on the self-consistent coupling of balance equations for optical and acoustic phonon baths with the Monte Carlo simulation of the electron Boltzmann equation. To investigate the electric, thermal and thermoelectric properties of ultra-thin Si layers, Neophytou et al. have coupled the linearized Boltzmann transport theory with a tight-binding model for electronic properties and with the Valence-Force-Field method for the calculation of the thermal properties. Sevinçli et al. have used an atomistic NEGF approach to investigate the impact of disorder on both electron and phonon transport in carbon nanotubes. As a function of the length of the disordered structure, they show the coexistence of different regimes of transport, i.e. quasi-ballistic, diffusive and localization regimes. The results suggest that disorder can be an effective mechanism of engineering the thermoelectric properties of carbon nanostructures. Finally, to study the carrier dynamics under electromagnetic excitation in two-dimensional electronic systems, Sule et al. have combined in an original way the Ensemble Monte Carlo (EMC) method for carrier transport with finite-difference time-domain (FDTD) technique for electrodynamics and Molecular Dynamics (MD) for short-range Coulomb interactions among particles. They apply this approach to calculate the dc and ac conductivity of graphene layers supported on silicon oxide substrate for different impurity distributions. Larcher et al. present a comprehensive approach that describes charge transport and degradation phenomena in high-k stacks. It is based on a

self-consistent simulation of charge transport (dominated by the defect-assisted contribution), power dissipation and temperature increase, defect generation, and ion and vacancy diffusion and recombination. It is shown to reproduce accurately several effects like the stress-induced leakage current, the threshold voltage shift observed during positive bias temperature instability stress, the threshold voltage increase and time to breakdown in various dielectric stacks.

The issue contains also a lot of papers that describe different ways to implement multiscale approaches. Two of them propose to connect atomistic to continuum approaches and even several levels up to circuit simulation. Auf der Maur et al. review different ways of coupling atomistic-based quantum mechanical simulation approaches with classical models. They focus in particular on the problems of strain, electronic properties and electronic transport in devices within the TiberCAD framework. Gerrer et al. describe a generalized multiscale approach to investigating the reliability of circuits. It starts with molecular dynamic and Density-Functional Theory (DFT) simulation to describe oxide traps. The results are injected in device simulation from which a compact model library is extracted including impact of oxide degradation. This model is then used to analyze the failure rate in elementary circuit cells.

Another trend of multiscale simulation consists in combining information coming from different levels for a better understanding of a particular problem. Rudan et al. have developed such an approach dedicated to the charge transport in Ovonic chalcogenide materials and devices. It includes modeling levels ranging from simulations of nanostructures of simple geometry to the simulation of technologically relevant device structures by means of general-purpose device-simulation tool. Nier et al. investigate the mobility in high-k metal gate Ultra-Thin Body and Box Fully Depleted SOI devices with the support of experimental data. They demonstrate an excellent agreement between Non-Equilibrium Green’s Function (NEGF) and Kubo-Greenwood (KG) solvers, and then use extensively KG data as a reference for the accurate calibration of TCAD model parameters for different scattering mechanisms.

The multiscale simulation may also starts from first-principle calculation. Blom et al. show that if the detailed physics of interfaces at the atomic scale is usually considered at the first-principles level, in nanodevices they start to play a dominating role, and need to be treated as an active part of the device, and not just as an invisible boundary between different materials. Saha et al. extend the use of DFT simulation to the device level with more than two electrodes in the NEGF approach. They give an overview of this new trend in computational electronics and apply their method to study the transport between a graphene nanoribbon and a carbon nanotube, showing an effect of negative differential resistance. To study the screening effects on conductivity of

graphene in graphene-dielectric heterostructures, Kharche et al. have developed an approach combining DFT calculation and the classical image-potential model. They investigate the effects of screening from surrounding materials like h-BN, SiC, SiO₂, Al₂O₃, and HfO₂ on the dielectric function and charged impurity scattering limited conductivity of graphene.

Albareda et al. have developed an efficient quasi-analytical self-consistent and time-dependent algorithm of boundary conditions for electron device simulators. The algorithm is shown to be robust, requiring limited computational efforts and suitable for any classical or quantum electron device simulator for both stationary and dynamic (transients, noise and AC) regimes up to several THz.

A multiscale strategy may also be developed to validate a simplified and pragmatic approach from results of more sophisticated simulation. Torrente et al. describe two different algorithms based on the statistical field-impedance method to calculate the random telegraph noise amplitude statistics in nanoscale MOS devices. The two schemes, based on either an approximation on doping or an approximation on traps, are thoroughly discussed. To show their validity the results from these schemes are compared successfully with results of Monte Carlo simulation, known to be more accurate but more computationally demanding. Bufler et al. have developed an accurate quantum correction model for 3D Monte Carlo simulation of MOS transistors. This quantum-correction can be extracted from a 2D cross-section of the

3D device and remains accurate also for short-channel devices. It is a multiscale approach in the sense that long-channel results (2D cross-section simulation corresponds to 3D long-channel simulation of the sheet density) are shown to be applicable to short-channel device simulation, as in the examples of FDSOI devices and FinFETs with a gate length of 15 nm. Frégonèse et al. have built an improved compact model of graphene transistors. As a validation step, they carefully compare the different features of their model with results of NEGF simulation. The model is then used to design a mm-wave amplifier operating at 140 GHz.

Finally, two groups describe their multiscale simulation packages which are made available to the community. Baumgartner et al. present the Vienna Schrödinger-Poisson (VSP) simulation tool. It includes models for band structure calculation, self-consistent carrier concentrations including strain, mobility, and transport in transistors and heterostructure devices. Its capabilities are demonstrated via the examples of tri-gate and nanoscale planar transistors, quantum dots, resonant tunneling diodes, and quantum cascade detectors. Fonseca et al. present the current state and new functionalities of the tool NEMO5, including advances in quantum transport simulations and with materials such as metals, topological insulators, and piezoelectrics. This software implements a broad range of atomistic models such as the Schrödinger equation and non-equilibrium Green's functions (NEGF) in tight-binding formalism, for electronic structure and transport calculations, respectively.