Advanced physics for simulation of ultrascaled devices with UTOXPP solver

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Abstract

As the conventional scaling down of MOSFET dimensions faces physical and economical limits, the performances obtained with novel technology options such as new dielectrics, mechanical strain and substrate orientation or alternative device structures, must be evaluated within the perspective of an industrial integration. State-of-the-art physically-based models for band structures, quantum tunneling and charge trapping have been implemented into a Poisson-Schroedinger solver. The effects of material alloys band structures, heterostructure and strain on the electrostatics and quantum transport can be investigated. A multi-phonon assisted non-radiative trapping model is used to study the impact of defects on device reliability and trap-assisted tunneling.

Keywords: Poisson–Schroedinger model, TCAD modeling, full–band model

INTRODUCTION

The downscaling of MOSFET dimensions has been a very successful process in improving the performances of CMOS devices as more and more aggressive ITRS requirements are targeted [1]. Conventional scaling down of MOSFET dimensions faces physical and economical limits. The performances of novel solutions such as high-K dielectrics, mechanical strain and substrate orientation, or alternative device structures, such as fully depleted SOI devices, must be evaluated within the perspective of an industrial integration. The effects of these technological boosters on channel mobility and gate leakage have to be clearly quantified.

In state-of-the-art commercial TCAD device simulators [2], quantum effects are accounted for using the Density Gradient approximation, that well applies to traditional bulk devices, but risk of being inaccurate for advanced devices such as SOI structures. Moreover, emerging materials significantly challenge the conventional TCAD tools due to the lack of appropriate empirical model parameters calibration.

Among the new technological boosters of advanced devices, it is now well established that applied mechanical strain and channel orientation in substrate engineering can significantly improve carrier mobility. Moreover, alternative architectures, such as multi-gate MOSFETs and Fully-Depleted Silicon-On-Insulator (FD-SOI) devices are emerging. In addition, new materials and process steps need to be added to the manufacturing process flow at every new technological node.

A successful modeling approach should combine conventional TCAD simulation tools with physically-based models. The investigation of physical phenomena and the calibration of empirical models implemented in commercial TCAD tools can be performed in this view. In response to the industrial need, new physically-based models have been developed in the academic world. However, their application to industrial environment is rarely effective due to their limited versatility, portability, support and user-friendly interfaces.

In this work, a new TCAD modeling tool is proposed for the investigation of advanced quantum effects, band structure models, quantum tunneling and multiphonon-assisted charge trapping.

SOLVER AND GUI DESCRIPTION

State-of-the-art physically-based models featuring advanced tunneling models, band structure effects, and mobility calculation have been implemented into a Poisson - Schroedinger solver (UTOXPP).

In Figure 1, the features of the modeling tool are presented. The core of the model is represented by a 1D Poisson-Schroedinger solver. Full-band k.p and multi-band EMA models are used to calculate the material bandstructure of up to six different materials [3] [4]. This makes possible the investigation of heterostructure and strain effects present in modern devices and nanoscale technologies. The user has the possibility to calibrate the material parameters on more rigorous simulations, and a specific set of electrical and band structure parameters has been extracted from ab-initio studies for the common materials adopted in CMOS. In the full band models, the oxides have been treated as pseudo zinc-blende materials, adjusting the model parameters to match the band structure obtained from first principles [5] [6].

Semiclassical WKB and quantum tunneling models have been integrated for the calculation of the tunneling current through oxide stacks. An accurate determination of the barrier transmission in complex stacks requires the use of inelastic Non Equilibrium Green Func-

tion (NEGF) techniques [7], while a semi-analytical approach based on the WKB approximation can be adopted for simpler barriers [8]. A multiphonon-assisted non radiative trapping model has also been included and permits to accurately calculate the response of interface and oxide defects after electrical stress and extract the trap distribution in oxide layers [9].

The tool is used for DC, AC and transient analysis on CMOS devices. Additional features include charge predication techniques to improve numerical convergence and reduce the simulation time on multicore CPU clusters. Multi-threading capabilities and job scheduling have also been included.

Given the complexity of the included physical models, where often the definition of a large number of parameters is required, a graphical user interface has been implemented to improve the user-friendliness of the tool. The interface, based on Qt C++ and OpenGL libraries, also makes possible the generation of high definition plots for reporting purposes. Some screenshots of the interface have been illustrated in Figure 2 and all the plots presented of this paper have been created with it.

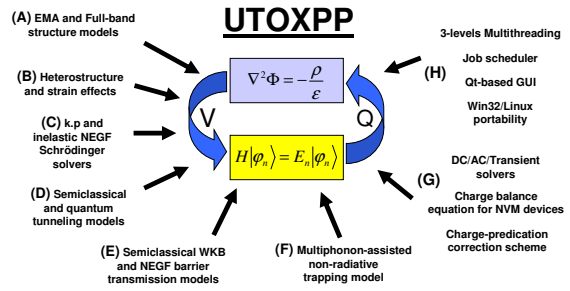

Figure 1: Building blocks of UTOXPP.

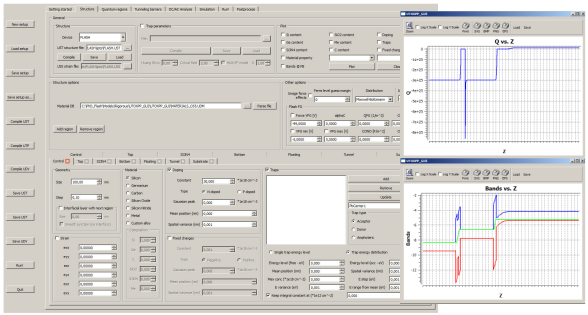

Figure 2: Screen-shot illustrating the UTOXPP graphical user interface which has been implemented to improve the user-friendliness of the tool. Portability is for both Win32 and X11 Linux/Unix systems.

BAND STRUCTURE MODELS

Typical outputs of UTOXPP are presented in the following. Figures 3(a-c) show the calculated silicon band structure for h^+ using a 6-band k.p model for different lattice orientations. A 30-band k.p model taking into account electron spin can be used for the calculation of the band structure for e^- (Figure 3(d)). These results can be used for the extraction of simpler band structure models suitable for compact approaches. Effective mass approximations (EMA) models have been calibrated in proximity of the confinement valleys Γ and Δ on the previously shown results. They are commonly adopted for electrical device simulations to reduce the computation effort (Figures 3(e-f)). Additionally, strain effects on the bands can be taken into account and modeled in EMA and k.p using the analytical S of the Bir-Pichus model at Γ [4]. The band structures of unstrained/strained germanium calculated with the 6-band k.p model are also shown in Figure 4.

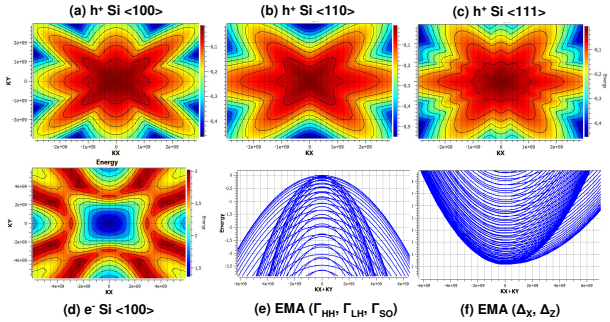

Figure 3: (a-c) Calculated silicon band structures for h^+ for different lattice orientations using the full band k.p model. In (d), silicon band structure calculated for e^- taking into account 30 bands with the full band k.p model. In (e-f), band structures of the Δ and Γ valleys in the effective mass approximation.

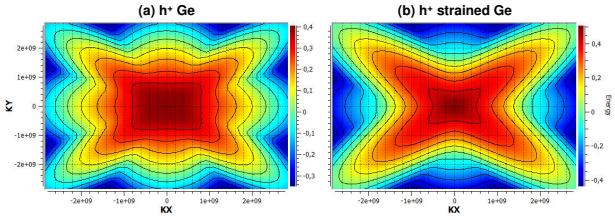

Figure 4: Germanium band structures calculated using the 6 bands k.p model for h^+ for unstrained (a) and biaxially-strained (b) material.

DEVICE SIMULATIONS

UTOXPP permits the electrical simulation of conventional and state-of-the-art devices. In the following some examples are provided to illustrate the functionalities of the tool. Figure 5 shows the calculated band diagrams of four archetypal structures, namely a conventional NMOS device, a HKMG strained PMOS device, a fully-depleted SOI NMOS structure and a 65nm NVM flash device. The rigorous calculation of the band structure, the potential profile and the charge distribution performed with multi-band models can be used both for TCAD analysis of physical phenomena and compact models validation. For device in Figure 5(d), the floating gate voltage has been simulated taking into account an iterative approach for the solution of the charge balance equation [10].

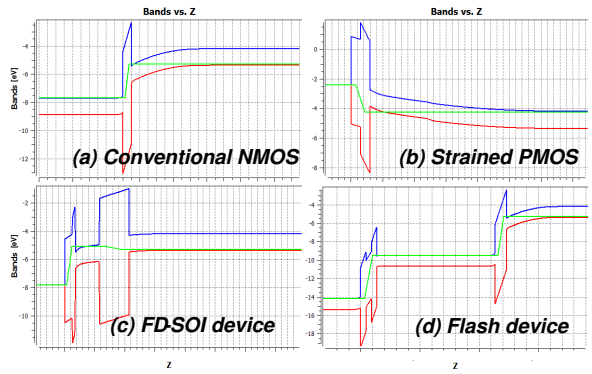

Figure 5: Band structure diagrams of possible structures that can be simulated with UTOXPP: conventional MOS structures (a), advanced devices with novel oxide stacks (b), FD-SOI devices (c) and flash memory cells (d). Blue: conduction band, red: valence band, green: quasi Fermi level.

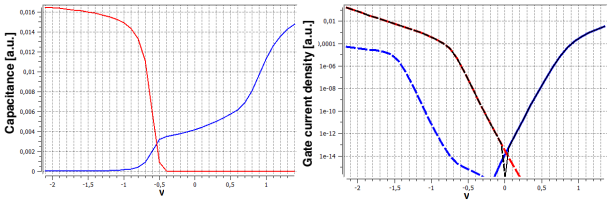

Figure 6: Gate capacitance (a) and leakage current density (b) calculated for the device in Figure 5(b). The h^+ (red) and e^- (blue) components can be identified.

Electrical simulations are used to determine the gate capacitance and the tunneling currents through energetic barriers. In Figure 6(a), the split capacitance of the PMOS device presented in Figure 5(b) is shown. The effects of the strained layer and of the wave function penetration into the HK oxide stack are taken into account [6]. Both stress type and quantification, substrate orientation and structure composition effects on the equivalent electrical oxide thickness can be determined in an accurate way. Figure 6(b) shows the tunneling current vs. gate bias voltage through the oxide barrier of the same device. In this plot, the semiclassical WKB approach has been adopted for the calculation of the tunneling transmission.

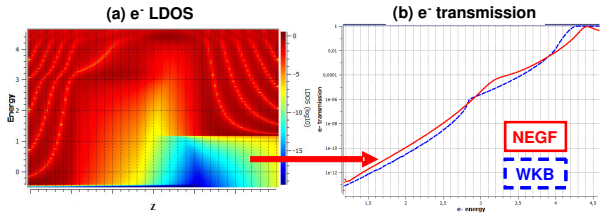

Figure 7: (a) Local density of states (LDOS) of e^- in accumulation, calculated for the device in Figure 2(b) using the NEGF solver. The quantum approach also permits to compare the barrier transmission with a semiclassical WKB approximation (b).

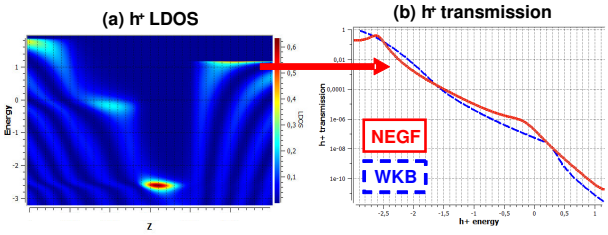

Figure 8: Same as in Figure 7 for h^+ in strong inversion.

Figure 7(a) and Figure 8(a) show the local density of states (LDOS) vs. position in the same PMOS device calculated using the NEGF solver for both accumulation e^- and inversion h^+. This model, benefits of the multithreading capabilities of the tool for the parallelization of the calculation in energetic levels. Figure 7(b) and Figure 8(b) compare the evolution of the barrier transmission vs. energy determined with the WKB model and the NEGF solver for e^- and h^+, respectively. Quantum oscillations linked with the resonance of the states are visible at the top and at the bottom of the barrier. In HKMG stacks, resonances are also present in the HK layer due to the bandgap variation.

A multiphonon-assisted charge trapping model has been integrated to accurately determine the impact of interfacial and bulk defects in oxide stacks. The model has been presented in detail in a previous publication [9] and is suitable for DC, AC and transient analyses, with

different approaches for the solution of the trapping rate equation.

The defects capture/emit carriers with a frequency depending on their energy and position into the oxide layer (Figure 9(a) for the PMOS device in Figure 5(a)); the capture and emission rates calculated with the multiphonon theory are exponentially decreasing for traps placed deeper in the oxide and in the energy gap. The frequency-dependent parasitic trap capacitance shown in Figure 10 can be calculated from the intrinsic frequency distribution and using an AC small signal model [9]. The parasitic trap admittance is taken into account in the calculation of the total gate capacitance and conductance as a function of small signal frequency and bias voltage (Figure 10). The model can be used for the extraction of the trap concentration distribution in the oxide stacks and at the substrate interface.

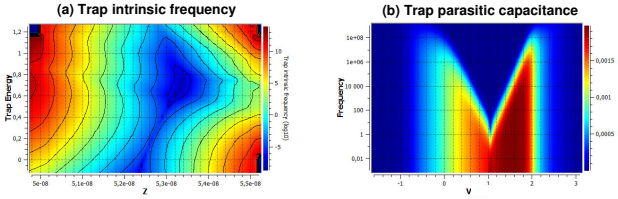

Figure 9: Intrinsic trap frequency as a function of defect energy and oxide depth, determined with the multiphonon approach. It represents the rate of communication of the defect with the reservoirs and indicates the range of defects that can be characterized at a given AC frequency. As traps respond with an intrinsic capture/emission frequency (a), they cause an additional bias and frequency dependent parasitic capacitance (b).

CONCLUSION

A new TCAD modeling tool including advanced models for band structure and device simulation has been presented. It permits the investigation of the effects of technological boosters commonly used in advanced nanoscale CMOS technologies, the evaluation of quantum confinement and tunneling in complex heterostructures, the investigation of band structure deformation and device electrostatics in strained alloys and of impact of defects in oxide layers with a rigorous multiphonon approach. Including both a DC, AC and transient model, it permits to perform device simulations in most of the device operating conditions and can be used for validating or extracting simpler empirical models based on compact approaches. The graphical user interface strongly improves the user-friendliness and portability of the tool, while efficient techniques have been adopted for multithreading and parallel calculation.

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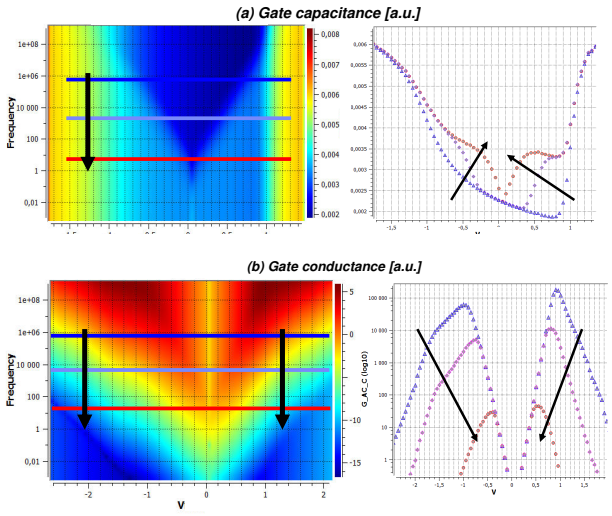

Figure 10: Gate capacitance (a) and conductance (b) for a fairly degraded SiO_2/Si interface as a function of applied gate voltage and AC signal frequency. The cuts are shown for 3 frequencies (lines), clearly indicating the impact of traps on the device impedance. The CV distortion increases with decreasing frequency as low frequency signals are able to scan the electrical signature of traps with lower capture/emission rates. The total concentration of traps at the interface is $2.05 \cdot 10^{12}$ cm^{-2}.

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