

ICT Project no. 258547

ATEMOX

Advanced Technology Modeling for Extra-Functionality Devices

Publishable Summary Second Period























Project summary and objectives

Within previous European projects with major contributions by the current partners, process simulation has been brought to a state which allows in industrial environments a sufficiently accurate simulation of doping profiles in advanced CMOS technologies. Important electrical characteristics of core CMOS devices can now be predicted from scratch or with a minimum calibration effort.

However, concepts towards low-power electronics, smart power applications, CMOS image sensors, and CMOS derivatives providing extra functionalities are still not sufficiently supported by TCAD. This concerns especially the prediction of leakage currents in such or parasitic devices caused by electrically active defects that remain after processing, and alternative doping techniques like plasma immersion ion implantation, low-temperature implantation, diversified cocktail implants and laser annealing which are considered for low-leakage ultra shallow junctions. The lack of suitable models that can be used in the early stages of industrial R&D inhibits the necessary cost reduction in the development of devices for which Europe is still at the forefront. Our project will develop the full set of missing models and implement and include them into the Sentaurus TCAD platform of Synopsys so that they are of immediate value to the European semiconductor industry. The integrated models will finally be evaluated by STMicroelectronics with respect to industrial needs.

To reach these ambitious goals, a consortium of European companies active in complementary fields of competence (STMicroelectronics: device manufacturing, Synopsys: TCAD software, Exico, IBS: equipment production, Probion, Semilab: characterization) and leading European research institutes (CNRS-LAAS/CEMES, CNR-IMM, ETH-Zurich, Fraunhofer-IISB, Univ. Newcastle) has been formed which, together, is well prepared to expertly cover all fields from experiment via characterization and modelling to simulation.

The ATEMOX consortium

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Centre national de la recherche scientifique	France
Consiglio Nazionale delle Ricerche	Italy
Eidgenössische Technische Hochschule Zürich	Switzerland
Excico France	France

Ion Beam Services
Probion Analysis SARL
France
Semilab Felvezeto Fizikai Laboratorium Reszvenytarsasag
Hungary
STMicroelectronics Crolles 2 SAS
France
STMicroelectronics S.A.
France
Synopsys GmbH
Germany
Synopsys Switzerland LLC
Switzerland

University of Newcastle upon Tyne

United Kingdom

Work performed and results achieved

For high-k dielectrics, physical effects were reviewed and suitable candidates for the inclusion into TCAD software were identified. For high-k dielectrics, improved Monte-Carlo parameters and analytical tables were developed, too. A study by Z. Essa et al. on the evaluation and modelling of lanthanum diffusion in TiN/La₂O₃/HfSiON/SiO₂/Si high-k stacks was presented at the E-MRS Spring Meeting, Strasbourg, France, May 14-18, 2012

Based on a large experimental library of STMicroelectronics featuring pre-amorphization and cocktail implants, the limitations of existing continuum diffusion models were investigated. This has resulted in a new selection of models for nitrogen co-implants and a comprehensive calibration of the Sentaurus Monte Carlo model for amorphization by ion implantation. The work with SIMS data has been complemented by an investigation of limitations in the theoretical basis of existing continuum diffusion models and by ab-initio and classical molecular dynamics calculations. One of the potential improvements investigated is a transition from 'compact' to 'extended' point defects at high temperature, having the effect of a temperature dependent activation energy and entropy of diffusion. Figure 1 illustrates one type of extended point defect investigated by molecular dynamics calculations – a small amorphous pocket that might be stabilized by misfit strain.

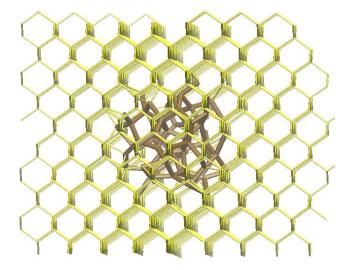


Figure 1: Structure of a 'monointerstitial' amorphous pocket computed by molecular dynamics

To simulate the redistribution of dopants during melting laser annealing, physical models and simulation strategies have been pursued by the consortium. The work allowed ruling out out-diffusion and migration in a temperature gradient as main contributions. Possible explanations include a two-species approach in the liquid phase as well as the assumption of an accumulation by segregation at the interface between the liquid and the solid phase. Figure 2 shows simulation results for the latter model in comparison to experiments. The results of the work were presented at the E-MRS Spring Meeting, Strasbourg, France, May 14-18, 2012 (G. Fisicaro et al.) and at the 19th International Conference on Ion Implantation Technology, Valladolid, Spain, June 25-29, 2012 (G. Fisicaro et al, M. Hackenberg et al.).

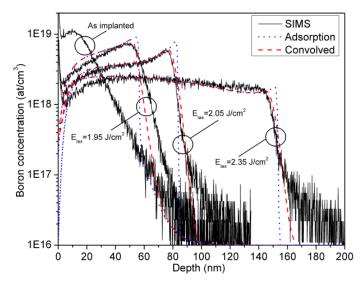


Figure 2: Simulated profiles using the adsorption model and convolved profiles resulting from a simulation of the SIMS measurement conditions compared to the SIMS measurement.

For the simulation of plasma immersion ion implantation (PIII), state-of-the-art experiments were carried through and modelling strategies were investigated for Monte-Carlo methods and analytical approaches. As an example, Figure 3 shows a comparison of a 1 keV BF3 plasma implantation profile to simulations with the Monte Carlo ion implantation tool of Sentaurus Process using an appropriate energy distribution of various boron-containing species in the plasma. In the experimental investigations, as in the example of Figure 4, a prominent pile-up of boron was found below the a/c interface and could be successfully simulated by a model taking boron trapping at end-of-range defects into account. The results of the work were presented at the 16th International Conference on the Simulation of Semiconductor Processes and Devices, September 8-10, Osaka, Japan (A. Burenkov et al.) and at the 19th International Conference on Ion Implantation Technology, Valladolid, Spain, June 25-29, 2012 (F. Cristiano et al., Z. Essa et al., A. Burenkov et al.).

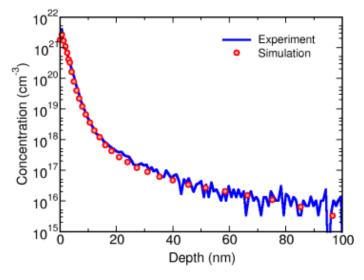


Figure 3: Comparison of a 1 keV BF₃ plasma implantation profile to simulations with the Monte Carlo ion implantation tool of Sentaurus Process

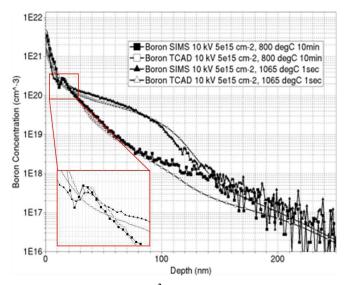


Figure 4: SIMS vs. TCAD for a BF³ 10 kV ion implantation after annealing.

As an important part of the ATEMOX work, the electrical properties of interstitial clusters were investigated in advanced structures. As an example, Figure 5 shows DLTS spectra measured after ion implantation of silicon and appropriate annealing to invoke the formation of self-interstitial clusters. In further work, the data will be correlated to junction leakage measurements. The results of the work were presented at the 19th International Conference on Ion Implantation Technology, Valladolid, Spain, June 25-29, 2012 (C. Nyamhere et al.).

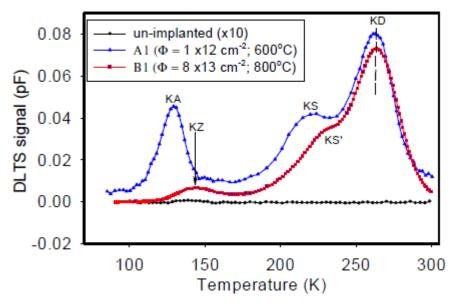


Figure 5: DLTS spectra measured after ion implantation and annealing

Based on the DLTS and leakage current data, the development of generation-recombination models for extended defects started. A simplified, compact, and robust trap-assisted tunnelling model was derived and ported to the "Traps" module of the device simulator Sentaurus-Device of Synopsys. This allows studying the impact of different spatial trap distributions. Generically defined defect concentration profiles resulted in IV-characteristics similar to those of the poly finger diodes provided and measured by ST Crolles. The observed broadening of the DLTS peaks calls for the development of models for distributed trap energy levels

and inter-level recombination traffic. This will lead to an extension of the coupled-defect level model in Sentaurus-Device.

A physics-based model for N diffusion and N cluster formation has been included in the Advanced Calibration set of models and parameters for Sentaurus Process F-2011.09. The model allows studying the impact of N co-implant on USJ formation.

A model for dopant redistribution during SPER (solid phase epitaxial regrowth) has been calibrated and integrated into the Advanced Calibration set of models and parameters for Sentaurus Process G-2012.06. Its robustness has been successfully tested in applied 1D and 2D simulation of USJ formation processes.

Amophization of silicon by ion implantation has been investigated for most implantion species used in device manufacturing. The calibration of the corresponding amorphization models has been integrated into the Advanced Calibration set of models and parameters for Sentaurus Process G-2012.06.

Expected final results and potential impact

The project is expected to lead to a quantitative understanding and the establishment of quantitative models in a variety of fields of process and device simulation that far exceeds the current state-of-the-art.

In the area of process simulation, progress beyond state-of-the-art is expected especially for critical processes and alternative doping processes considered for the fabrication of CMOS derivatives with well-controlled on-characteristics and leakage currents:

- Diffusion phenomena observed during processing at low temperatures, such as out-diffusion or in-diffusion of dopants at temperatures below 850 °C
- Dipole formation, interdiffusion, and dopant diffusion through high-k dielectrics
- Extended cocktail implants involving co-doping of arsenic and phosphorus and eventually carbon for n+ regions, activated by spike annealing and non-melt laser annealing
- Extended cocktail implants involving combinations of boron, fluorine, and carbon for p+ regions, activated by spike annealing and non-melt laser annealing
- Melting-laser processing
- Plasma immersion ion implantation
- Ion implantation at elevated and cryogenic temperatures

In contrast to previous work on doping processes for main-stream CMOS applications, progress will not only be achieved for activation and diffusion, but also for the formation of electrically active defects with deep levels in the band gap.

In the area of device simulation, progress beyond the current state-of-the-art will be achieved for the modelling of leakage currents, in particular leakage currents caused by process-induced defects.

Currently, a deficiency in the capabilities of TCAD, namely the insufficient calculation of leakage currents, prevents its usage for the design of increasingly smaller CMOS derivatives for which objectives from low dark currents to low consumption are as important as performance. With the successful achievement of the objectives of this project, European semiconductor industry will be able to save considerably development time and costs as for the core

CMOS technologies by using TCAD early in the design of CMOS derivatives so that the respective electronic components and systems may be offered earlier and cheaper to the market. With the potential of TCAD to save about one third of the development time and costs also for CMOS derivatives as documented in the ITRS, the expected commercial potential of our proposal is substantial.

Project web site

http://www.atemox.eu

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