Introduction

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As many other technological fields, the fabrication and design of new integrated circuits (ICs) make intensive use of Technology Computer-Aided Design (TCAD) tools. The goal of process modeling is to provide physical understanding and simulation tools to help the development and optimization of device fabrication. Simulation tools are used in the different steps of the fabrication chain from equipment-related issues to fundamental material properties. The information resulting from process modeling (device geometry, dopant distribution, defect concentration, etc.) is then used as input for device simulation to predict the electrical device behavior, which in turn is used for compact circuit simulation and system modeling. Therefore, the accurate modeling of the physical effects of manufacturing steps used to build transistors is key within a successive hierarchical modeling framework for the development of new ICs. The International Technology Roadmap for Semiconductors (ITRS) provides the guidelines for the development of semiconductor devices in different aspects. A whole chapter devoted to modeling and simulation indicates its relevance in the semiconductor industry. Process modeling and simulation are becoming fundamental to reduce development times and cost of new technologies, allowing a fast and extensive exploration of processes and materials, and providing understanding to experimental data and, thus, clues for optimization.

Progressive device downscaling has allowed a higher level of integration in ICs with improved cost/performance ratios. Semiconductor technology is evolving not only to build more miniaturized transistors in ICs (*More Moore*)

but also to provide ICs with enhanced functionalities (*More-than-Moore*). This evolution entails a number of technological challenges that are also translated into process simulation requirements. Modeling capabilities must evolve to encompass processes, equipment, geometries and materials considered for present and future devices. Scaling of transistors demands not only higher degree of accuracy but also may require new models for new effects or effects that were neglected in previous technology nodes. The extension of silicon technology outside the conditions traditionally used to make transistors (solar, power, imaging, sensors, MEMS, etc) requires to validate models and parameters outside the range for which they were initially established, as well as to develop models for new materials and structures.

Continuum models continue being the mainstream in industry for process simulation because they are fast and can be easily coupled to device simulators. Nevertheless, the reduction of device dimensions and the augmented computer power have given atomistic techniques a key role, both as direct simulation approaches and as a pathway to improve continuum models. Ab initio methods are also acquiring more relevance because the lack of free parameters makes them very useful tools for exploring new materials.

Process modeling is greatly concerned with junction formation. Therefore, the accurate prediction of dopant distribution and activation during the fabrication processes is one of the main goals of process modeling. Most challenging is the formation of ultra-shallow junctions, which has driven the exploration of molecular, cold or cocktail implants and the transition from furnace anneals to other anneal schemes such as spike rapid thermal processes and millisecond anneals. Excimer laser annealing has also been considered for the healing of crystal damage and activation of dopants in particular structures.

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At materials level, much attention is devoted to defect evolution as they control the point defect supersaturation, which in turn affect dopant redistribution. Lattice defects may also induce energy states in the gap responsible for current leakage. Interactions among defects and dopants must be modeled in detail as they greatly determine dopant diffusion and activation through the diffusion of mobile species and the formation and dissolution of various types of impurity clusters. The presence of high stresses to enhance charge mobility should be also considered in process simulation since it affects the equilibrium concentration of point defects, the effective dopant diffusivities and also the dopant solid solubilities. The incorporation of other materials to substitute Si in the channel, such as Ge or III-V compounds, is promoting a number of studies to establish models and parameters in these materials during the process flow.

This special issue on Process Modeling contains a collection of nine invited papers which overview the state-of-the-art and the challenges that face process modeling as it accompanies technology development. The selected papers cover different aspects of process modeling and evidence the complexity of the physics involved. They illustrate the need for both atomistic and continuum models to construct hierarchical schemes to take advantage of each technique strengths.

The paper by Lorenz et al. gives an historical perspective of some important achievements on the understanding of material science for applications in process modeling, as well as the challenges for new technologies from the perspective of the ITRS guidelines. The paper also deals with modeling issues in the area of lithography, layer deposition and etching processes. A hierarchical scheme that include modeling at equipment level to identify the main sources of device variability is also presented.

The contribution of Cea and his team offers an interesting review on the state-of-the-art of front-end process modeling and poses perspectives for future technologies. They describe how atomistic and continuum methods are combined to model modeling geometry, doping and stress effects in advanced logic processes.

The paper by Noda et al. covers the main aspects of modeling ultra-shallow junction formation, which involves phenomena like amorphization, defect evolution dopant diffusion and clustering, both for n-type and p-type regions.

The paper by Aboy and coworkers provides a comprehensive description of dopant-defect interactions, with emphasis on boron and Si interstitial defects. They examine the influence of the parameter setting to describe the mechanisms involved in process modeling in a broad technological window.

The paper by Zographos and Martin-Bragado offers a comprehensive model of the stress and chemical effects in SiGe alloys. Models for amorphization, dopant diffusion and clustering, defect evolution, etc are revised and additional effects such as band-gap narrowing or SiGe inter-diffusion are also considered.

Modeling of excimer laser annealing requires a complex modeling that includes the coupled simulation of the electromagnetic field, for the calculation of the heat source distribution, and the simulation of the thermal phase and impurity fields for the prediction of the material modification. The paper by Fisicaro and La Magna reviews all these aspects, and presents a link between continuum models and Kinetic Monte Carlo method for the detailed modeling of dopant-defect interactions in the rapidly changing thermal field.

Although many features of process modeling for the silicon solar cell fabrication are common to those involved to build transistors, there are some differences and sensitivity to parameters. The contribution by Florakis et al. is devoted to modeling of doping and defect removal strategies in crystalline silicon solar cell. It points out the relevance of oxidation models, and long time furnace anneal to create deep profiles compared to ultra-shallow junctions required in transistors.

The paper by Aoki shows molecular dynamics simulations of cluster impacts on solid targets, with direct technological applications in ion implantation and etching. He considers effects of ion penetration, sputtering and crater formation associated to relatively small clusters of boron or carbon, and huge clusters of argon or fluorine.

The paper by Nordlund and Djurabekova describes a multiscale modeling framework to model irradiation in nanostructures. They review different atomistic techniques, the physics involved, their advantages and limitations for modeling nanoscale phenomena and illustrate some examples of their use.

In spite of the intensive research and effort during decades to develop predictive models for the various aspects related to IC processing, there are still many unknowns and the field is far from being settled. It is a challenge to gather all the information needed for predictive process modeling in time should new materials, architectures and processes become relevant ingredients in future technologies. Nevertheless, the explosion of computer resources at an affordable price contributes to the rapid progress in process simulation. Calculations that were prohibitive a decade ago are now affordable and open interesting possibilities for process simulation.