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Multiscale modeling of doping processes in advanced semiconductor devices

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ABSTRACT

The development of advanced semiconductor devices relies heavily on technology computer-aided design. Front-end process simulators model the fabrication of devices including different process steps and effects such as ion implantation, dopant and defect diffusion and interaction, epitaxial growth, and stress effects. Continuum process simulators continue to be the main tool; however, kinetic Monte Carlo simulators with and without lattice have become important as well. With the need to explore new materials other than silicon, such as SiGe, germanium, and III–V, more fundamental modeling is required to compensate for missing experimental information. *Ab initio* methods based on density functional theory and molecular dynamics can help address open questions of material characteristics that cannot be extracted explicitly by experiments. In this paper, we give an overview of a multiscale approach for advanced process modeling and discuss the latest progress.

1. Introduction

Technology computer-aided design (TCAD) for semiconductor device development and manufacturing has been used by the semiconductor industry and academia for many years. It helps to understand the underlying physics needed to improve device performance and to enable device manufacturability. TCAD can be separated into two key aspects: process simulation for virtual device fabrication and device simulation for virtual device operation.

In this paper, we will focus on process simulation for doping processes in advanced semiconductor devices. Many detailed reviews of process modeling can be found in the literature, for instance, for front-end Si in general [1], for continuum process modeling in particular [2], and for process modeling for advanced device technologies [3,4]. Therefore, we concentrate on recent achievements and new trends where Synopsys has been involved.

Now as in the past, TCAD has mainly been applied in the device development phase. Process simulators, mainly continuum ones, are calibrated based on experimental data, in particular, secondary ion mass spectrometry (SIMS) and sheet resistance data, and on electrical data of specific devices, and then the process simulators are used for device development and optimization. Recently, there has been a new trend to apply TCAD in the exploration phase of devices and processes involving new materials. Whenever a new material or a new chemistry is introduced to semiconductor process technology, a new model or a new calibration of an existing model is needed. Although experiments have been and will be the basis of modeling and calibration, it is challenging to establish useful models using experimental measurements only because of the ever-increasing complexity of materials, processes, and models, as well as the lack of useful experiments or devices. Obviously, this requires more predictive physical models that need less calibration. One way to achieve this is involving more and more physics-based models, in particular, atomistic ones.

Physics-based modeling offers the following advantages:

- It is relatively predictive.
- It provides insight into physics and chemistry that would be otherwise inaccessible.
- It provides a portal to theoretical knowledge in a way that is more accessible to non-experts.
- It is much quicker and cheaper than performing experiments.

Atomistic models describe the behavior of atoms. Continuum models describe the behavior of a continuum unit cell. Models at this scale disregard the discrete particle-based structures of the material, in this case, semiconductors such as SiGe, Ge, and InGaAs. However, based on the size and scale of modern CMOS devices, continuum modeling remains the workhorse for efficient modeling of the behavior

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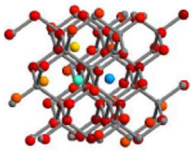
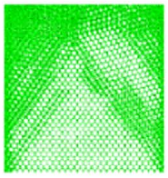
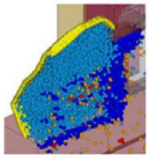
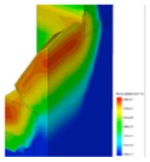
Modeling Technique	Visualization	Structure Size	Times Simulated	CPU Time
Ab initio		~10^2 atoms	~10^{-2} ns	Slowest
Classical molecular dynamics		~10^5 atoms	~1 ns	
Lattice kinetic Monte Carlo		Part of device	Part of process	
Kinetic Monte Carlo		Complete device	Complete process	
Continuum		Complete device	Complete process	Fastest

Fig. 1. Summary of physics-based modeling techniques for process simulation and their characteristics.

and characteristics of such devices within practical timescales.

In the following, we discuss several important modeling methods, describe their advantages and limitations, and elaborate on some application examples.

2. Methods

Each simulation technique provides information at a different scale level and, therefore, is a useful module in a hierarchical multiscale scheme. Fig. 1 summarizes various modeling techniques and their characteristics.

Ab initio techniques such as density functional theory (DFT) are based on the solution of the Schrödinger or Dirac equation and can extract information on the electronic properties of the material. *Ab initio* can be considered the most fundamental atomistic technique since it gives insight into the underlying physics of semiconductor materials with no free parameters. It can yield information about defects and dopants, and their interaction mechanisms. *Ab initio* has been used extensively in Si technology to study the formation energies of point defects and dopant-defect clusters, as well as diffusion mechanisms and diffusion barriers. Many *ab initio* studies use simulation cells of 64 or 216 atoms.

The computational overhead of *ab initio* arises from the resolution of the Schrödinger equation. One possible simplification involves sacrificing this electronic description and calculating the effective influence of the electrons over the atoms through an analytical expression, called an *empirical potential*. Empirical potentials must be explicitly designed to properly describe the properties of the materials in the system under study (for example, Si, Ge, and InGaAs). If a new system will be studied, a new parameterization or even a new analytical expression must be developed, which is not straightforward. Molecular dynamics (MD) simulations using empirical potentials are commonly called classical molecular dynamics (CMD). They have been used for energetic and structural characterization of Si self-interstitials, vacancies, and small interstitial clusters in Si, as well as for studying self-diffusion.

Kinetic Monte Carlo (KMC) techniques refer to off-lattice kinetic Monte Carlo algorithms, meaning that the lattice is discarded (in contrast to lattice KMC), and only the defects in the simulated crystal are tracked. This technique is designed to simulate the dynamics of a system for time intervals comparable to real processing times. The KMC technique is a statistical approach in which random numbers are used to determine the events that occur, the particles that are involved, and the interactions involved based on the underlying physics of the system. For small devices, KMC can model complete process flows. The main difficulty in the implementation of new models in KMC is determining the interactions and events that are relevant and the parameters that govern them. It is worth noting that many parameters involved in the kinetics of impurities and defects, such as binding and migration energies, and emission/capture rates of extended defects, are impossible to extract from direct experimental observations. At this point, *ab initio* techniques can help to identify and characterize the relevant mechanisms and the associated energies.

Lattice kinetic Monte Carlo (LKMC) is a KMC technique suited to simulate the three-dimensional growth of the exposed interfaces of a crystal by a one-by-one incorporation of atoms into such interfaces.