Introducing Monte Carlo Diffusion Simulation into TCAD tools

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ABSTRACT

Advantages and disadvantages of the alternative approaches to the dopant diffusion simulation are discussed. Complementary use of the Monte Carlo and continuum diffusion models is suggested. Application of the integrated commercially available process simulation tools DADOS (atomistic) and Taurus Process (continuum) to the advanced sub-100 nm devices is demonstrated.

The following four application areas for the Monte Carlo diffusion model are discussed: 1. Determining model parameters for the continuum process simulation. 2. Complete Monte Carlo path from implantation to diffusion for investigating statistical device variations. 3. Usage of DADOS integrated into Taurus Process for the accurate diffusion simulation in the entire simulation domain or a small window in the most critical device part. 4. Exploration of the new materials and species for the novel devices and process steps.

Keywords: Monte Carlo, diffusion, process, simulation, TCAD.

1 INTRODUCTION

Predictive simulation of doping processes remains the focus of process simulation for sub-100 nm devices. The shrinking thermal budget significantly reduces diffusion and therefore, reduces the need to accurately model diffusion.

However, much more complex dopant activation and deactivation phenomena do not reach thermodynamic equilibrium during the thermal annealing and their understanding and characterization become increasingly important. The dynamics of point defect configurations and interaction with the dopants need to be modeled accurately to predict active doping profiles and device performance.

Traditionally, dopant diffusion and activation phenomena are simulated using TCAD tools based on the continuum approach. An emerging atomistic approach to the diffusion modeling represents dopants and defects as discrete particles rather than continuous concentrations. Let's analyze the benefits and applicability ranges of the two approaches.

2 DIFFUSION: CONTINUUM AND MONTE CARLO APPROACHES

2.1 Limitations of the Continuum Approach

Despite their importance, the density of the point defect and dopant-defect clusters is often quite low and their gradients are very steep, such that their representation by a continuous average concentration becomes questionable.

As it is currently understood the number of different configurations of point defects and dopants that need to be accounted for is rather large. Their binding and activation energies vary significantly, in particular for the small clusters with less than a dozen atoms.

In the traditional continuum approach based on solving a system of partial differential equations (PDEs), a separate balance equation needs to be solved for each of these species. Both the fitting of the large number of parameters required by such systems and the solution of these large, highly non-linear and tightly coupled systems of PDEs, as well as ordinary differential equations (ODEs) and algebraic equations require a significant amount of computational resources.

2.2 Complementary Monte Carlo Approach

A Monte Carlo based diffusion simulation may provide a valuable alternative to the continuum approach. It is usually easier to implement more detailed physics models into the Monte Carlo model compared to the continuum model. The main disadvantage of the Monte Carlo approach is the extremely high computational resources that it requires for the large simulation domains.

While we expect the well-established PDE models to be much more efficient than the Monte Carlo models for 1D and 2D simulations, the sub-100 nm devices have a number of inherently 3D effects, and therefore, increasingly require 3D simulation. The need for 3D simulation and shrinking device sizes drastically reduces the CPU time gap between the two approaches. The recently reported CPU times for the kinetic Monte Carlo diffusion simulations [1] look very promising compared to 3D PDE simulations for realistically complex sets of equations on sufficiently fine meshes.

The Monte Carlo methods are already successfully used for the simulation of ion implantation. The binary collision codes capture very well the traditional materials and implanted ions for the silicon technology and readily extend to new combinations of target materials/implanted ions. Empirical damage models allow to predict the amount of channeling of doping profiles for a broad range of energies, doses, tilt and rotation angles. The most sophisticated binary collision models simulate the full cascades of knock-on lattice atoms in complex 2D and 3D geometries.

These models do not however predict the damage configurations and size distributions of point defect/dopant aggregates at the end of the ion implantation. The modeling of damage anneal, cluster formation, and diffusion tails during implantation can be done using Monte Carlo diffusion simulation.

3 INTEGRATING CONTINUUM AND MONTE CARLO METHODS

3.1 DADOS

The kinetic Monte Carlo simulation package DADOS has been developed over the last several years and has been used to study and understand the fundamental physical phenomena in silicon [1]. DADOS contains powerful diffusion modeling capabilities, but lacks complicated geometry, multiple materials and interfaces, and moving boundaries. For the full understanding of the impact of the highly accurate Monte Carlo physics models on the transistors it is mandatory to account for the full interaction of all involved materials and surfaces in the device structure that is evolving during the fabrication steps.

Realistic applications require simulation of the entire process flow, including implant, etch, deposition, anneal, oxidation, epitaxy, and silicidation steps. Simulation of these processes is well established in the commercial TCAD tools. Integrating such a PDE-based simulator with a Monte Carlo simulator allows to combine accurate geometry representation, stress distribution, dopants, defects, and dopant-defect clusters and their evolution during the entire process flow.

At the same time it adds new challenges to the Monte Carlo diffusion simulation, both to the physical models used e.g. for modeling of the interaction at material interfaces or the self-consistent accounting for the electric field, and to the fundamental data structures and related algorithms. While we feel that a rigorous ab-initio calculation will remain beyond the computation power and time resources of even our most advanced TCAD users, we sense the demand in the advanced TCAD user's community to increasingly use Monte Carlo diffusion capabilities in the near future. To satisfy such a demand, we have generalized the DADOS data structure and geometry representation capabilities, and integrated it with the 1D/2D/3D continuum-based process simulator Taurus Process [2].

3.2 Applications

One of the fundamental applications that we expect to use DADOS for is to extract parameters for the models to be used in the continuum-based simulators. Another possibility is to use DADOS directly interfaced with Taurus Process for the deep submicron device simulation. In this case DADOS can be either used for the entire simulation domain from Taurus Process or only for a small window in the most critical part of the device.

Let's look at one of the end-of-roadmap devices where the continuum approach breaks down, whereas the atomistic approach has its full strength. Figure 1 shows the 20-nm nMOSFET at the end of the process flow simulated using 3D Taurus Process.

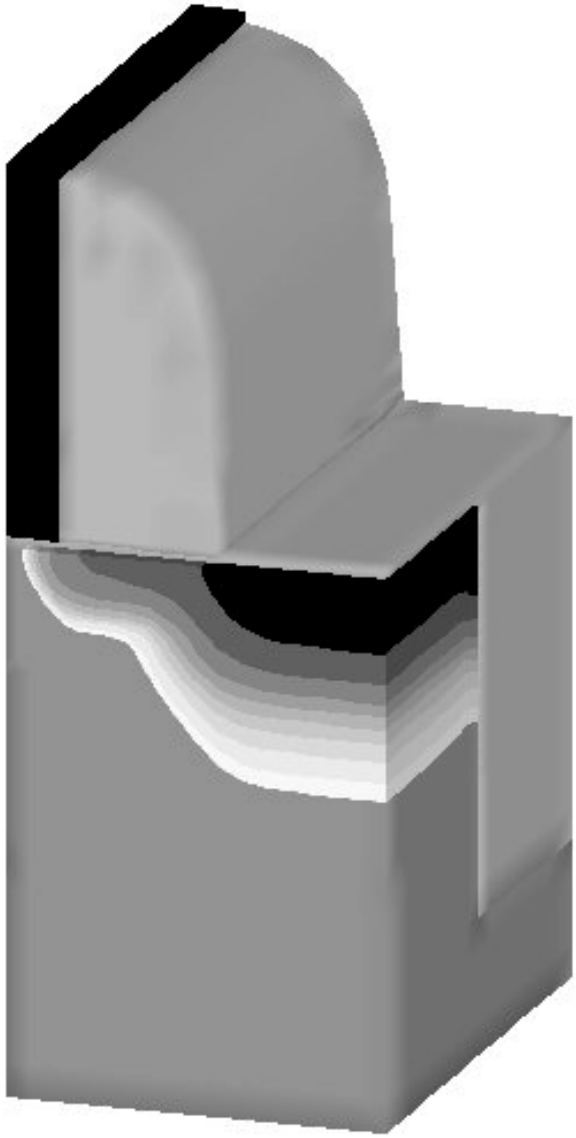

Figure 1: 3D simulation of a 20-nm nMOSFET. The final arsenic profile is shown in the source/drain region.

Figure 2 shows the 2D projection of the 3D DADOS simulation domain (100x50x70 nm^3) after the extension and high dose arsenic implants. The light color depicts silicon self-interstitials, while the darker color shows vacancies. The arsenic atoms are completely hidden under a much higher concentration of the implant damage.

The vacancies dominate near the silicon surface, and interstitials dominate deeper into the substrate, while at the arsenic channeling tail the interstitials and vacancies are intermixed rather uniformly.

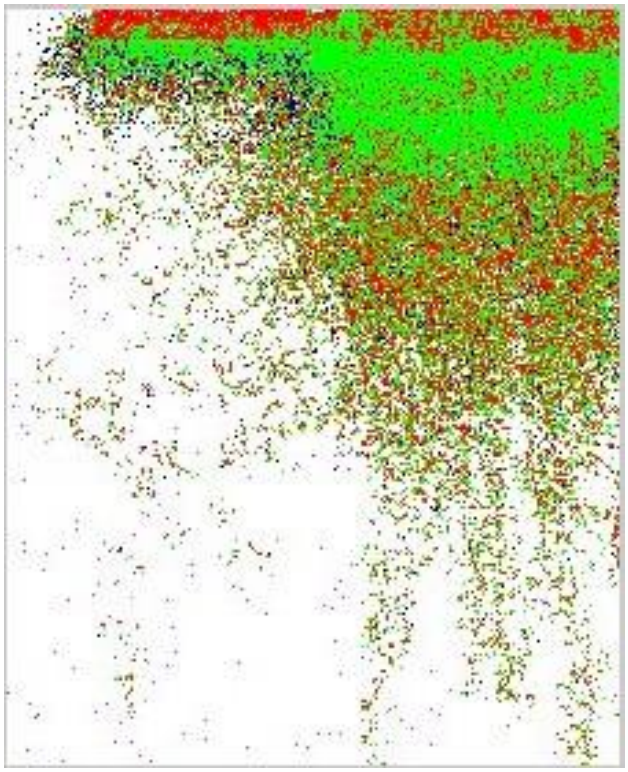

Figure 2: 2D projection of the 3D simulation domain with as-implanted arsenic profile after the extension (3 keV, 10^{14} cm^{-2}) and high dose (10 keV, $4 \cdot 10^{14}$ cm^{-2}) arsenic implants.

Figure 3 shows the structure after 1 second anneal at 950°C. Several {311} extended defects are clearly visible under the high arsenic concentration area. Both individual interstitials and vacancies are gone at this point, and only {311} and arsenic atoms are present.

Figure 4 shows the structure after the entire source/drain activation anneal of 15 seconds at 950 °C. The structure is reflected about the center of the MOSFET channel to show both source and drain profiles necessary for device simulation.

The {311} extended defects have completely disappeared by the end of the anneal and only arsenic atoms are visible.

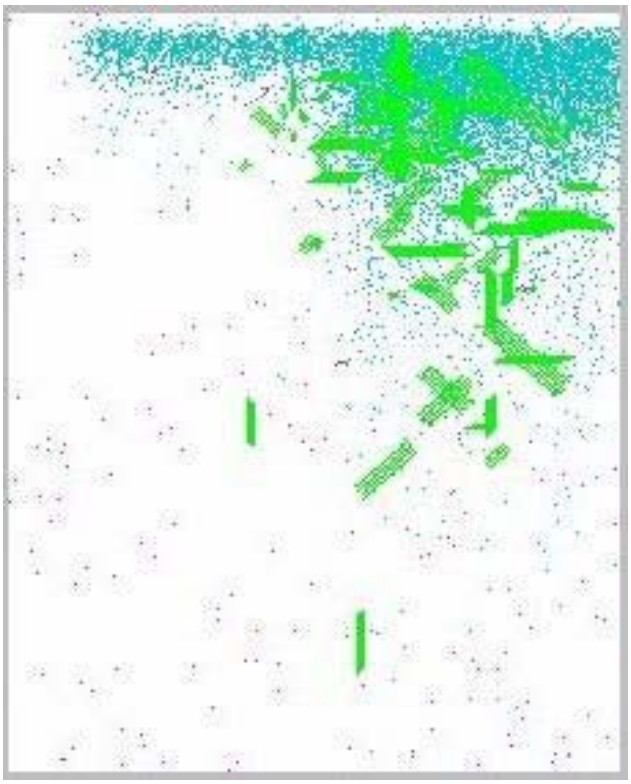

Figure 3: Source/drain profile after 1 second anneal at 950°C.

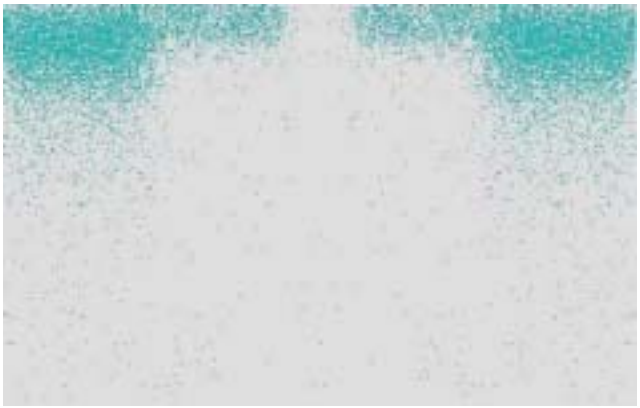

Figure 4: Source and drain profiles after 15 seconds anneal at 950°C.

It is obvious that the effects due to the discrete nature of dopants and defects are not accounted for in the continuum simulation. DADOS simulation was performed including all possible reactions and configurations of the dopants and defects. The entire 3D simulation took 32 minutes on a 450 MHz Pentium-II CPU.

The third application field that we foresee for the atomistic diffusion modeling is to combine the Monte Carlo implant and Monte Carlo diffusion models, which opens a possibility to directly investigate statistical variations for

the devices with a small number of dopant atoms in the active regions. This is becoming an increasing concern for the small device dimensions [3].

The fourth possible application area is discussed in the next section.

3.3 Exploring New Materials

During the past few years the semiconductor research community is performing intensive search for the new materials and new processing approaches to bypass some limitations of the conventional silicon processing. These materials/fabrication steps are much less understood compared to the traditional processes like thermal silicon oxidation.

The traditional model development cycle, from deriving appropriate mathematical models at a university or research lab, publishing the results, until the numerical implementation in a commercial code and quantifying all necessary model parameters is becoming a bottleneck for the use of the TCAD tools in general.

To gain predictive power for yet unknown materials and process variations a different and much more flexible approach is required to provide modeling insight tailored to the specific processes and material combinations of a TCAD user. This flexibility is required particularly during the investigation of alternative materials and development of novel process steps, but equally important is the immediate availability of the new models by all engineers of a manufacturer's TCAD group.

This duality of the requirements of maximum tool flexibility for the research needs and maximum robustness for the mass production applications will be addressed by the new generation of TCAD tools, combining the benefits of atomistic and continuum approaches.

4 CONCLUSIONS

Analysis of the alternative approaches to modeling dopant diffusion in silicon shows that the conventional continuum method can be successfully complemented by the novel kinetic Monte Carlo method. The capabilities of the integrated commercially available TCAD tools DADOS and Taurus Process are demonstrated on an end-of-roadmap device.

We expect that the atomistic Monte Carlo diffusion approach will be increasingly used in the semiconductor industry. The shrinking device dimensions demand higher accuracy of physical models and drastically reduce the simulation domain size, bringing the required computational resources down to the practically acceptable range.

Considering that the atomistic diffusion modeling is a new and rapidly evolving field, we anticipate that it will pose serious challenges, but it will also open new horizons in understanding future semiconductor materials and processes.

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