Multiscale Modeling and Simulation of Semiconductor Processing:
Application to ultrashallow junction fabrication in Si

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Technology computer-aided design (TCAD) models have been extensively employed in the semiconductor industry to improve the efficiency of development as well as production. Thus far, many phenomenological models for key processes including dopant implantation/annealing have been developed. However, the validity of those conventional continuum-based models becomes questionable as devices scale down to the 100 nm node. Below 100 nm, greater fundamental understanding and knowledge of materials and physical processes are necessary for defining device processing. Nonetheless the availability of reliable fundamental data is limited due to the difficulty of measurements during actual processing. Under such circumstances, it becomes important to develop a comprehensive hierarchical theoretical model built on quantum mechanics. The multiscale modeling will offer tremendous opportunity in not only improving current technology but also forecasting future device manufacturing.

We have applied the multiscale approach to uncovering complex phenomena occurring during the fabrication of ultrashallow junctions with high concentrations of dopants. The formation of ultra-thin and low-sheet-resistance $pn$ junctions are necessary for higher performance transistors. To achieve a precise control of junction properties it is necessary to understand quantitatively (i) underlying mechanisms of transient enhanced diffusion (TED) of dopants and (ii) dynamics of defect-dopant clustering during implantation and postimplantation annealing. For this study we have developed a multiscale model in which we combine (i) kinetic Monte Carlo and continuum-based simulation of relatively long-time scale phenomena such as defect-dopant clustering/dissolution and doping profile evolution with (ii) quantum mechanics [density functional theory] simulation of the fundamental microscopic processes. I will present (i) new mechanism of B TED, (ii) pathway of boron clustering associated with Si self interstitials, and (iii) the results of doping profile evolution simulations for various process conditions, together with experimental validation.
Figure 1. Issues in ultrashallow junction fabrication.

- $B^+$ implantation (< 1keV)
- Gate electrode
- Oxide
- Source
- Drain
- Si
- Annealing (~ 1000 °C)

Process requirements
- maximize dopant activation
- minimize dopant diffusion

Better understanding of
- ion implantation
- dopant diffusion
- defect-dopant interactions

Development of predictive numerical models

Figure 2. Multiscale modeling of ultrashallow junction processing.

- Experiments: ultrashallow junctions
- prediction
- validation
- Continuum mechanics:
  - Doping profile evolution
- Reaction information
- Kinetic Monte Carlo:
  - Defect-dopant dynamics
- Fundamentals data
- Quantum mechanics:
  - Microscopic processes

B concentration, cm$^{-3}$

0 200 400 600 10$^{10}$ 10$^{18}$ 10$^{20}$ 10$^{21}$ Depth, Å

Experiment
Simulation