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THE SUMMARY OF Ph.D. DISSERTATION

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Title

Advanced Process Modeling Research for sub-100nm CMOS

Abstract

A new set of modeling and simulation methods for sub-100nm CMOS fabrication processes including ion implantation and dopant diffusion, was developed. Our simulation models enable us to perform precise MOSFET process/device coupled-simulation including "reverse short channel effect", and to obtain new insights for intrinsic fluctuations of sub-100nm MOSFET characteristics.

Detailed dopant distribution profile calculation is critical for a practical application of TCAD (Technology Computer Aided-Design). Most conventional simulation tools are based on the fitting models due to insufficient understanding of physical phenomena. In this work, we have investigated some new simulation methods including an atomistic way to ensure high accuracy and predictive capability of the simulation analyses.

Chapter 1 summarizes the background and previous studies.

Chapter 2 describes a model for ion implantation simulation considering a silicon crystal structure. A scattering calculation scheme based on a modified binary-collision-approximation was improved for reproducing channeling tails of implanted ion distribution profiles. Our statistical enhancement method and parallel computing, achieved 100 times faster calculation. A simulation method of SIMS was also investigated for accurate shallow junction profiling.

Chapter 3 describes the modeling for post-implantation diffusion and electrical activation simulations. Both continuum and atomistic modeling approaches were examined. Boron and Arsenic diffusion models were improved based on the point-defect/dopant pair diffusion model, and the new models can be used to reproduce reverse-short-channel-effect that is caused by source/drain implantation damage in conjunction with non-equilibrium pair-diffusion kinetics. In addition, we have developed kinetic Monte Carlo diffusion simulation scheme considering detailed boron /interstitial complex formation mechanism and charged species. Fundamental model parameters such as formation energy or binding energy values were taken from *ab initio* calculations and molecular-dynamics (MD) simulation results. This MC diffusion simulation enables us to perform "predictive" analysis for short-time (spike) annealing processes.

In chapter 4, using atomistic process simulation tools developed in this study, intrinsic statistical fluctuations in sub-100nm device characteristics were examined associating 3D atomistic device simulations. Gate line-edge-roughness (LER) and random discrete dopant distribution effects were incorporated in these simulations. The simulation analyses also revealed that some diffusion-less annealing processes such as the extremely short time annealing technique would increase the fluctuation arising from LER. This atomistic process simulation enables us to obtain non-trivial insights that will be useful in further optimizing the design of fabrication processes.

Chapter 5 summarizes the results of this study.