SUMMARY OF Ph.D. DISSERTATION

School Fundamental Science and	Student Identification Number	SURNAME, First name SHIMIZU, Yasuo
Technology		
Title		
Experimental Study of the Behavior of Point Defects and Dopants in Silicon		
using Isotope Superlattices		

Abstract

Advancement of silicon (Si) complementary metal-oxide-semiconductor (CMOS) device performance has relied on scaling. It has progressed so much that the present accuracy requirement has reached less than 1 nm for the spatial control of source/drain regions. A typical fabrication process of source/drain regions is composed of ion implantation of dopants, followed by annealing to electrically activate the implanted species. In the previous generation of micrometer CMOS, separation distances between the source, gate, and drain were large enough to neglect the effect of defects coming from one region to the others for modeling of the entire fabrication process. However, the separation distances in today's nano-CMOS are so small that defect formation, migration, and their chemical reactions in a particular region can significantly affect the formation process of the other regions. Understanding the behavior of host Si atoms is becoming increasingly important for the precise control of both dopant diffusion and activation.

This study reports the nanoscale investigation of host Si behavior related closely to the control of the source/drain fabrication processes in advanced CMOS. In particular, 1) determination of Si self-diffusivity below 875 °C and identification of the microscopic picture of self-diffusion, 2) determination of Si displacement lengths induced by collision with ion-implanted dopants and criteria for amorphization by implantation, and 3) evaluation of time-dependent Si self- and dopant diffusion enhancement by excess Si point defects created by ion implantation (transient enhanced diffusion) were performed experimentally. Moreover, complete numerical modeling of each process has been achieved for process simulation.

Investigations of the behavior of Si atoms in the matrix of Si crystals have been extremely challenging. In this study, successful growth of isotope superlattices (SLs), composed of alternating atomic layers of different stable isotopes (²⁸Si and ³⁰Si), has led to simultaneous observations of the behavior of dopants and Si atoms after ion implantation and annealing using the different masses of Si isotopes as markers. In Study 1), Si self-diffusion was induced by annealing of the isotope SLs, and the resulting smearing of the mass distribution was detected as changes in the phonon frequencies by Raman spectroscopy. Si self-diffusivities for 700-900 °C were determined precisely and it was found that the vacancy dominates self-diffusion in this temperature range. In Study 2), Si displacements were evaluated quantitatively by secondary ion mass spectrometry (SIMS) probing the smearing of the periodic depth profile of ³⁰Si in the isotope SLs induced by ion implantation. Further analysis involving cross-sectional transmission electron microscopy revealed that amorphization occurred when our displacement parameter exceeded ~ 0.5 nm. This critical value was found to be independent of the implanted ion, energy, and dose. In Study 3), transient enhanced diffusion of boron and ³⁰Si in boron-implanted isotope SLs were observed by SIMS. Their time-dependent depth profiles were reproduced successfully by numerically solving rigorous diffusion and chemical reaction models that were developed.

Some parts of the above findings have already been implemented in commercial simulators used by semiconductor industries. The importance of understanding Si nanoscience is expected to grow along with the further advancement of Si electronics.