Electronic Structure of Condensed Matter

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Study on clustering of As atoms heavily doped in Si

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Introduction

Investigation of impurity atoms doped in very shallow region of Si crystals with high concentration is important for process technology for future large scale integrated circuits (LSIs). Electrical activation of the impurity atoms, in which they substitute lattice site of Si crystals independently, is necessary, however, some of them form clusters combined with vacancy defects in the host crystal and are electrically deactivated. Therefore, control of such impurity clustering is an important issue for scaled-down transistors used in LSIs because higher impurity concentration is required in the shallow regions. However, structures and distribution of impurity clusters depending on process conditions have not been clarified well.

In this study, As doped in Si substrates by using a current process technology for formation of ultra-shallow doped region are observed by EXAFS measurements.

Experimental

Si(100) wafers were doped with As by ion implantation with 3.0 keV up to a dose of 1.5×10^{15} cm⁻² followed by spike-rapid thermal annealing at 1050 °C. The depth profile of As concentration was measured by secondary ion mass spectroscopy (SIMS). The samples were etched with various depths (1-15 nm) by step-by-step etching, in which ozone oxidation and removal of the formed oxide layer were repeated [1]. An As doped bulk Si wafer (0.006-0.008 Ω cm) was also used as a reference.

EXAFS measurements for As were performed with grazing-incidence excitation with incident angle at around 5° and the As fluorescence signal was collected by means of the side-looking 17 elements Ge detector equipped in the beam line 9A and 12C.

Results and Discussion

The As concentration profile before the etching is shown in Fig.1, and etched depths of the prepared samples are also indicated overlapped on the profile corresponding to sample surfaces after the etchings.

Figure 2 shows Fourier transforms of EXAFS functions of samples with etched depth of 0 nm, 2 nm and 6 nm. Coordination of the first shell (\sim 2A) and the second shell (\sim 3.5A) was degraded at the surface (0 nm) but increased with the etched depth.

Figure 3 shows distances of the nearest neighbor, d_{NNN} , and those of the next nearest neighbor, d_{NNN} , as a function of the etched depth, based on the model in which an As atom substitutes a lattice site of Si crystal. It was found that the values of d_{NNN} were almost the same for all samples, while that those of d_{NNN} for shallow etched samples were smaller than that of reference sample and they recovered close to the value of the reference for deep etched samples.

From these results, in the near surface region shallower than 4 nm in which As concentration is higher than the solubility limit of As in Si, crystalline structure around the As atoms deviated from the diamond structure. It indicates probably that most As atoms form clustered structures in the near surface region. Further analyses with possible cluster models will be performed to reveal the cluster structures observed in this region.

Reference [1] K. Tsutsui *et al.*, J. Appl. Phys., 104, 093709 (2008). * ktsutsui@ep.titech.ac.jp



Fig.1 Concentration profile of As and etched depths of samples.



Fig.2 Fourier transforms of EXAFS functions of samples with etched depth of 0 nm, 2 nm and 6 nm.



Fig.3 Distances of nearest neighbor and next nearest neighbor as a function of etched depth.