Photoluminescence study of {311}defect-precursors in self-implanted silicon

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Abstract

Photoluminescence (PL) study using Ar laser revealed that {311}defect-precursors exist in the samples annealed at either 620 or 670 °C after silicon implantation. The peak energy shift from 0.94 to 0.90 eV is a direct evidence of atomic structural transformation from the smaller precursor interstitial clusters to {311}defects. The atomic structure of the precursor was investigated by using a first principle calculation program. The numerical calculation demonstrated that one of the most plausible structures for the precursors is the di-intersitital. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Annealing; Clusters; Defect formation; Ion implantation

1. Introduction

Ion implantation is a standard technique to form shallow junctions. However, it introduces excess Si self-interstitials, which subsequently evolve into {311}defects during thermal annealing. In the following annealing processes, interstitials released from {311}defects give rise to transient enhanced diffusion (TED) of dopants so that an accurate physical model of the formation and dissolution of {311}defects is essential to simulate TED of implanted dopants in IC fabrication processes. While the detailed structure and annealing kinetics of {311}defects have been considerably understood, very little is known about the nucleation of {311}defects. In this work, we have studied the transition from the smaller precursor interstitial clusters to {311}defects during thermal annealing with photoluminescence (PL) measurements and performed a first principle calculation to clarify the atomic structure of precursors.

2. Experimental method

Czochralski Si wafers with a boron concentration of 3×10^{17} cm^{-3} were implanted with 50 keV Si ions with fluence of 5×10^{13} cm^{-2}. Si ions instead of dopants were implanted to introduce excess Si self-interstitials into the Si wafers. After implantation, the samples were annealed at either 620 or 670 °C in nitrogen ambient in the time range of 1–810 min. PL measurements were performed at 10 K using the 476.5 nm line of an argon laser.

3. Calculation method

We investigated the possibility of di-interstitial as precursors of {311}defects by using ab initio calculation based on a generalized gradient approximation [1,2]. We used the efficient plane-wave ultrasoft pseudopotential code for Si lattice constant of 0.54 nm. Cutoff energy of electron wave functions in 64-atom supercells is 150 eV and $2 \times 2 \times 2$ Monkhorst–Pack k-point sampling was used.

4. Results and discussion

4.1. Experimental results

Fig. 1 shows PL spectra for the samples annealed at 670 °C for 1, 10, 90, 270 and 810 min. The relative

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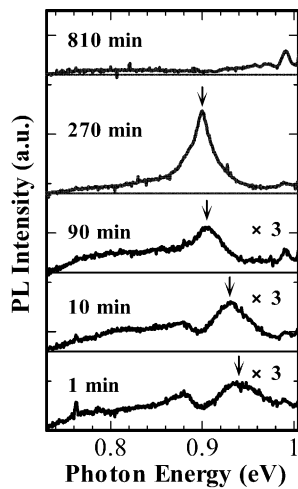*E-mail address:* tsuji@eie.eng.osaka-u.ac.jp (H. Tsuji).

Fig. 1. PL spectra from samples annealed at 670 °C for 1, 10, 90, 270 and 810 min. The symbol ' × 3'denotes the relative multiplication factor.
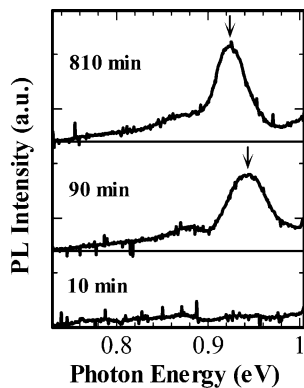

Fig. 2. PL spectra from samples annealed at 620 °C for 10, 90 and 810 min.

Fig. 3. {311}Defects-related PL peak energy as a function of annealing time.
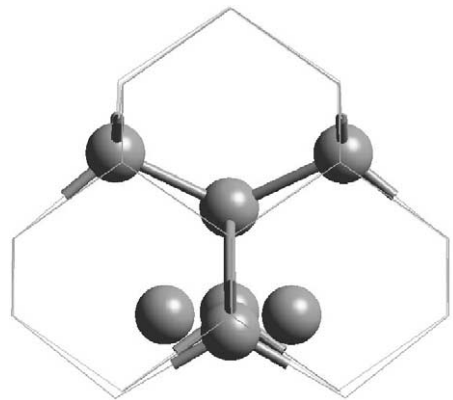
Fig. 4. Stable configuration of the di-interstitial in Si.

multiplication factor used for plotting is depicted on the right side in Fig. 1. A broad PL peak at 0.94 eV due to implantation damage is observed after annealing at 670 °C for 1 min as shown in the bottom of Fig. 1. As annealing time increases, the peak energy shifts continuously toward lower energy down to 0.900 eV after 270 min annealing which is associated with {311}defects [3].

Fig. 2 shows PL spectra for the samples annealed at 620 °C for 10, 90, 810 min. The broad PL peak at 0.94 eV is also observed in low temperature annealing at 620 °C for 90 min together with the shift of peak energy toward lower energy, as is the case of 670 °C annealing.

Fig. 3 shows the PL peak energy as a function of annealing time, which are indicated by the arrows in Figs. 1 and 2.

It should be noted that except for the samples annealed at 670 °C for 90 and 270 min annealing [4], no {311}defects were observed with high resolution TEM. These results strongly suggest that the smooth
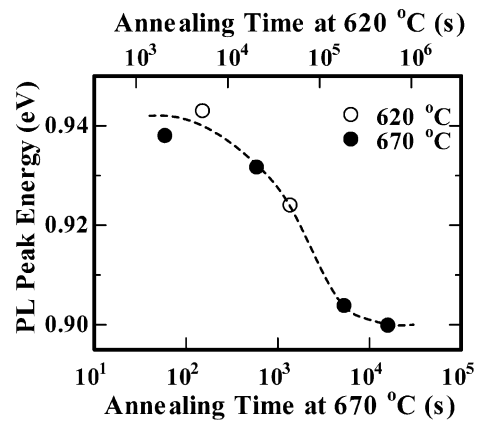
energy shift of the PL peaks is attributed to structural transformation from the smaller precursor interstitial clusters to {311}defects. In other words, the broad PL peak at 0.94 eV is associated with precursors of {311}defects. The peak shift toward lower energy may originate from the strain induced by defects [5] and/or associated with either growth or evolution of defects which lead to the reduction of the band gap. For more quantitative and detail discussion, more experiments would be required.

4.2. Calculation results

According to theoretical study of {311}defects, the di-interstitial [6,7] and the 4-intersitial cluster [8] have been considered as the precursor. We performed the ab initio calculations to investigate the possibility of the di-interstitials as precursors of {311}defects. We calculated the total energy in the system including two silicon atoms in Si lattice. In the calculation, two silicon atoms were placed at interstitial sites located around the center of the supercell with different initial atomic configurations.
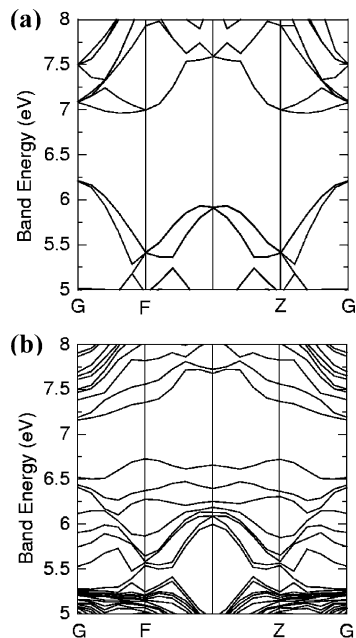
Fig. 5. Calculated energy band structures: (a) Si lattice; and (b) the di-interstitial based on ab initio calculations shown in Fig. 4.

Fig. 4 shows the most stable configuration of the di-interstitial. Fig. 5 shows calculated band-structure for crystalline Si (Fig. 5a) and Si lattice including the di-interstitial (Fig. 5b). It is obvious from Fig. 5 that reduction of the band gap is caused by the formation of the di-interstitial. This supports the idea that the broad PL peak at 0.94 eV is associated with precursors of {311}defects in the form of the di-interstitials.

5. Conclusions

The {311}defect-precursors have been investigated through photoluminescence measurements and ab initio calculations. We have found the broad PL peak at 0.94 eV which is presumably associated with precursors of {311}defects. The band-structure calculations support the possibility of the di-interstitials as precursors of {311}defects.

Acknowledgements

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