Photoluminescence study of self-interstitial clusters and extended defects in ion-implanted silicon

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Abstract

We report on the photoluminescence (PL) studies of self-interstitial (I) clustering in ion-implanted Si at various stages of post-implantation annealing. Low-temperature PL measurements on as-implanted and low-temperature annealed (up to 450°C) samples show sharp X and W bands at 1200 and 1218 nm which are attributed to I₄ and I₃ clusters, respectively. Annealing at 600°C shows a drastic change in the PL spectra. In case of high-energy self-ion-implanted samples, 600°C annealing produces several peaks in the range 1250–1400 nm. For longer duration annealing, two broad bands form at 1322 and 1392 nm irrespective of the ionfluence. These PL signatures are attributed to I₈ clusters and/or (100) I-chains, and they are believed to be the precursor of {311} rod-like defects. For annealing above 600°C and for fluence ≥1 × 10¹⁴ cm⁻², a sharp PL band is observed at 1376 nm and it is attributed to {311} rod-like defects. At higher fluences, an additional broad band appears in the PL spectrum at ~1576 nm which is related to residual ion-damage or extended defect formation. These results illustrate the potential of silicon I-clusters as a possible source of light emission from Si.

Keywords: Photoluminescence; Interstitial cluster; Defects; Silicon

1. Introduction

Implantation of energetic ions in semiconductors induces a variety of deep-level defects that are well characterized by electrical techniques such as deep-level transient spectroscopy. In contrast, an optical technique such as photoluminescence (PL) spectroscopy is comparatively less exploited in the study of deep-level defects. Despite a very low efficiency of luminescence in silicon owing to its indirect band gap, PL spectroscopy at low temperature has been an indispensable tool in the study of optically active defects in silicon for several decades [1]. A recent theoretical finding that stable interstitial (I) clusters in Si bound to dislocations may be responsible for dislocation-related PL [2] has opened up challenges for a deeper understanding of the electrical and optical properties of small I-clusters. Electrical signature and thermal stability of small I-clusters have been obtained recently [3]. Few studies have reported about the luminescence properties of {311} defect precursors [4,5], but no systematic studies have been attempted for small I-clusters in silicon. As these I-clusters are too small to be detected by electron microscopy, nondestructive optical
characterization of such defects is of immense importance for exploring their potential device applications.

In this article, we report on the PL studies on the growth and evolution of self-interstitial clusters in Si at various stages of post-implantation annealing. Low-temperature PL measurements were performed on keV and MeV ion-implanted silicon for a wide range of ion-fluence to identify the defects responsible for PL in silicon. It is shown that depending on the post-implantation annealing time and temperature, small clusters of interstitials and interstitial chains give rise to two distinct kinds of PL spectra.

2. Experimental details

The experiments were performed on epitaxially grown and Czochralski (CZ) grown n- and p-type silicon. Epitaxial n-Si samples were implanted at room temperature with 80 keV Al and Si⁺ ions at a fluence of $1 \times 10^{14}$ cm²⁻². CZ grown n- and p-type silicon samples were implanted with 1.2 MeV Si⁺ ions in the fluence range $1 \times 10^{13} - 5 \times 10^{13}$ cm⁻². Post-implantation annealing was performed under N₂ ambient in the temperature range 150–750°C for a duration of 30 min to 4 h. PL measurements were performed at 17 K using the 488 nm line of an argon laser.

3. Results and discussion

Fig. 1 shows a set of PL spectra recorded at 17 K on 80 keV Al⁺-implanted (fluence $= 1 \times 10^{14}$ cm⁻²) n-type Si subjected to post-implantation annealing at various temperatures for 1 h duration. The sharp peak W at 1218 nm corresponds to the well-known W band related to small I-clusters. W' band at 1237 nm is a phonon replica of the W band. The peak X at 1200 nm seems to be related to I-clusters, as it is independent of the implanted species and the impurity content of the Si wafer. The W line intensity attains a maximum for 300°C annealing, and at 450°C, W band intensity diminishes whereas X band intensity grows. This implies that X band is developed at the cost of W band, and the X band arises due to the formation of a bigger I-cluster at the cost of release of interstitials from smaller I-clusters responsible for W band. This feature was common to Si⁺-implanted samples as well. We studied (not shown here) the temperature and fluence dependence of these two bands and found that X band intensity grows with implantation temperature or post-implantation annealing whereas its intensity reduces with fluence. Due to the competing effect of nonradiative and radiative processes in ion-damaged Si, relative peak intensities cannot be used as a measure of the defect concentration. However, X band seems to anneal out at much higher temperature ($\sim 500°C$) than the W band as reported by Harding et al. [6]. In accordance with the previous studies, X band is attributed to I₄ clusters [7] whereas W band is attributed to I₃ clusters in Si [8].

Annealing at 600°C for 1 h shows a drastic change in the PL spectra. Al⁺-implanted samples show a broad peak I at $\sim 1340$ nm, and no W or X band were detected in Al⁺ or Si⁺-implanted. For Si⁺-implanted samples, 30 min annealing at 600°C induces a number of low-intensity PL peaks in the range 1250–1400 nm (not shown). At fluences $\geq 1 \times 10^{13}$ cm⁻², these peaks are not clearly identifiable, and they form two broad I bands at $1200$ and $1340$ nm.
\[ \sim 1322 \text{ and } \sim 1392 \text{ nm as shown in Fig. 2,} \]

irrespective of ion fluence and impurity content of Si wafers. The formation of these I bands after 600°C annealing only for the self-ion implantation implies that the respective bands are due to self-interstitial clusters whose size must be bigger than \( I_4 \). It can be noted that the width of the I band in this case is much larger than the width of the W or X band. A broad PL band may arise due to the strain surrounding the defect and corresponding broadening in energy level. Hence, a bigger but compact cluster or a (100) chain of interstitials may be responsible for these broad PL bands. In the literature, a similar defect signature has been attributed to the precursor of \{3 1 1\} defects \([4]\). Libertino and Coffa \([5]\) attributed similar peaks to the I-clusters in Si. As the proposed magic numbers for stable I-clusters are 4 and 8 \([9]\) and X band has been attributed to \( I_4 \) \([7]\), the observed I bands are likely to be related to the \( I_4 \) clusters and/or (1 0 0) I-chains. It can be noted that line width of the I bands are much larger than the line width of W and X bands. The occurrence of large line width in the PL spectra refers to the strain at/surrounding the defects. Hence, I-chains are more likely to be responsible for the observed I bands.

Fig. 3 shows the PL spectra of 1.2 MeV Si\(^+\) implanted (fluence = \(2 \times 10^{13} \text{ cm}^{-2}\)) n-type Si subjected to various annealing conditions. Annealing at 600°C gives rise to broad bands related to I-clusters. However, annealing at 680°C produces an intense peak R at 1376 nm, and broad peak D at \( \sim 1576 \text{ nm.} \) After annealing at 750°C, the R band intensity attains a higher value and the D band becomes very low. In the literature, the presence of R band is correlated with the growth of \{3 1 1\} defects in Si \([5]\). Hence, R band is attributed to the \{3 1 1\} rod-like defects whereas D band may be related to the residual damage. Our PL studies show that \{3 1 1\} defects are formed for a threshold fluence of \(1 \times 10^{13} \text{ cm}^{-2}\) and annealing temperature above 600°C. This feature is common to both p-type and n-type Si. In Fig. 4, we show a set
of PL spectra for p-type Si, where R band intensity attains a much higher value for 750°C annealing compared to the case of n-type Si. In p-type Si, damage-related broad band was not detected. Therefore, in case of n-type Si the observed broad band at \( \sim 1576 \) nm can be attributed to the recombination at the extended defects or confinement of carriers in the damaged zone.

4. Conclusions

Photoluminescence studies at low temperature for self-ion-implanted Si show a distinct signature of self-interstitial clusters of various sizes. Low-temperature annealing (up to 450°C) produces small clusters (I\(_3\) and I\(_4\) clusters) that are characterized by sharp PL bands at 1218 and 1200 nm, respectively. Higher temperature annealing (\( \geq 600°C \)) of self-ion-implanted samples shows a number of PL peaks in the range 1250–1400 nm related to I-clusters of various sizes. Annealing for longer duration induces two broad PL bands at 1322 and 1392 nm that are attributed to the bigger size I-clusters or I-chains. Finally, for fluence above \( 1 \times 10^{12} \) cm\(^{-2}\) and annealing temperature above 600°C a sharp and intense PL band at 1376 nm is observed and that is attributed to \{311\} defect. These studies show that Si interstitial clusters of various sizes are well detectable by the photoluminescence technique.

References