Photoluminescence Study on the Behavior of Self-Interstitials in Annealed Si Crystals

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1. Introduction

Oxygen precipitation takes place during annealing process of Czochralski(CZ)-grown Si crystals because of the presence of the supersaturated oxygen /1/. The oxygen precipitates produced by annealing at temperatures 600 - 1200°C consist of amorphous or crystalline SiO,
The volume of these precipitates is roughly two times as large as that of the corresponding Si atoms in the lattice. As a result, large stresses are induced at the precipitate/matrix interface. These stresses must be relieved by the emission of Si self-interstitials or by prismatic punching of dislocation loops. This concept is well-established /1/. Actually, the prismatic punched out dislocations have been observed in CZ crystals annealed at relatively high temperatures (T > 800°C). The appearance of extrinsic type stacking faults at annealing temperatures around 1000°C has also been explained by the same mechanism /2/. However, there have been no reports concerning the direct detection of Si self-interstitials.

The purpose of this work is to demonstrate the trace of Si self-interstitials using deep level photoluminescence (PL) spectroscopy. A strong and sharp line appears at 0.903 eV at certain annealing stages, regardless of the sources and the conductivity type of starting materials. The characteristic thermal behavior of the 0.903-eV line can be interpreted consistently assuming that the microdefects responsible for the line are correlated with Si self-interstitials.

2. Experimental

Conventional CZ-Si wafers (p-type, (100), p ~ 43 Q cm, [0] ~ 8.2 x 10^{17} cm^{-3} (DIN), [C] ≤ 1 x 10^{16} cm^{-3}) are subjected to isothermal anneal at 650°C for 1 - 450 h. In order to enhance the oxygen precipitation at this temperature, the samples are preannealed at 470°C for 64 h. The PL measurement of the samples at 4.2 - 77 K is performed in the photon energy range 0.7 - 1.2 eV.

3. Results

Figure 1 shows the PL spectra of the samples at 4.2 K. We will mainly pay attention to the deep level PL (0.7 < h < 1.0 eV). Before annealing, exciton luminescence appears in the band-edge PL but no signals in the deep level PL. An anneal at 650°C introduces a sharp and strong line at 0.903 eV as shown in Fig. 1 (b). This line consists of one main component at 0.9025 eV and four satellites with unequal spacings (Fig. 2). The intensity increases with annealing time in the initial stage, and after attaining a maximum at around 14 h it decreases gradually. If the annealing time is as long as 450 h, the 0.903-eV line becomes very weak and three broad bands appear at 0.81, 0.88, and 0.93 eV, as shown in Fig. 1 (c). The maxima of the three bands occur at the same energies as those of the so-called D1, D2, and D3 lines, respectively, which have been reported to be related to dislocations /3/.

4. Discussions

Infrared absorption studies show that the concentration of interstitial oxygen decreases with annealing time. Theoretically, one Si self-interstitial is emitted for two oxygen interstitials incorporated in the precipitate. Therefore, the concentration of Si self-interstitials increases with annealing time. However, if their concentration reaches a certain level, these Si self-interstitials begin to agglomerate, which results in the formation of interstitial-type dislocation loops. In fact, the rod-like defects, which are produced in CZ crystals by a long-time anneal at 650°C, have been identified to be interstitial-type dislocation loops /4/. Once these dislocations are formed, the concentration of Si self-interstitials decreases, since the dislocation loops grow larger by absorbing Si self-

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interstitials. Therefore, the concentration of Si self-interstitials first increases with annealing time, reaches a maximum value after a certain time, and then decreases. The expected concentration dependence of Si self-interstitials coincides with the intensity dependence of the 0.903-eV line. This leads us to conclude that the recombination centers responsible for this line involve Si self-interstitials. The appearance of the three broad bands after a long-time anneal is also consistent with the above model, if we assume that these bands originate in the dislocations forming the interstitial-type dislocation loops. The appearance of such a fine structure as in Fig. 2 does not contradict the present model, since many sharp lines have been observed in irradiated materials where interstitials, vacancies, and their complexes are created /5/.

5. Conclusion

The oxygen precipitation in CZ-Si crystals at 650°C introduces a characteristic PL line at 0.903 eV. The recombination centers responsible for the line involve Si self-interstitials either as single interstitials or in the form of small clusters.

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![Fig. 1. PL Spectra of CZ-Si crystals at 4.2 K. (a) as-received, (b) annealed at 650°C for 14 h, (c) annealed at 650°C for 450 h (with preanneal at 470°C for 64 h). Spectra are corrected for the PL system response.](image_url)

![Fig. 2. Highly resolved spectrum of the 0.903-eV line. The sample is identical to that in Fig. 1(b).](image_url)

![Fig. 3. Dependence of PL intensity on annealing time at 650°C for CZ-Si crystals with preanneal at 470°C for 64 h.](image_url)