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Microscopic and spectroscopic mapping of dislocation-related photoluminescence in multicrystalline silicon wafers

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Abstract Microscopic and spectroscopic photoluminescence (PL) mapping was performed on a region including intra-grain defects in multicrystalline silicon wafers in the temperature range between 15 and 300 K, and the temperature dependence of PL spectra from the region was studied. We confirmed that the origin of deep-level emission with an intensity maximum at 0.78 eV at room temperature was different from that of dislocation-related lines at low temperature. We believe that the 0.78 eV emission is associated with oxygen precipitation, and that the intra-grain defects are dislocation clusters decorated with not only heavy-metal but also oxygen impurities.

1 Introduction

High quality multicrystalline silicon (mc-Si) wafers have been required for fabricating higher-efficiency solar cells. The quality of the recent mc-Si wafers has been limited by the presence of intra-grain defects; therefore, analysis of these defects is important for improving the wafer quality. Dislocation-related lines (D-lines) [1] were observed in low temperature photoluminescence spectra from the regions which included the intra-grain defects [2]. These defects have been reported to be metal-decorated dislocation clusters which form small angle grain boundaries [3]. Deep-level emission located around 0.8 eV has been shown to appear in the defect areas at room temperature [4–6].

For further analysis of the intra-grain defects, we investigated the intensity distributions of the D-lines and the deep-level emission at about 0.8 eV. Then, we examined the temperature dependence of the PL spectra from the defect regions and identified the origin of the 0.8 eV emission.

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2 Experimental technique

The sample used in this study was a cast mc-Si wafer fabricated by a multi-stage solidification controlling method [7]. The wafer was boron doped with a resistivity of 2.5 Ω cm, a thickness of 270 μm and a size of 50 × 50 mm^2. The slicing damage was etched off by a HNO_3/HF solution.

PL spectra were measured in the temperature range between 4.2 and 300 K. The sample was excited by the 532 nm line of a ND:YVO_4 laser, which had excitation power and beam diameter of 6 mW and 1 mm, respectively. The PL from the sample was dispersed with a grating monochromator (Jobin Yvon HR320, f = 320 mm, F = 4.2) and detected by a Ge pin diode (North Coast EO-817L). The spectral response of the measurement system was calibrated with blackbody radiation.

PL microscopic and spectroscopic mapping were performed at temperatures from 15 to 300 K [8]. The laser beam was focused and scanned on the sample surface with a diameter of 10 μm and a scanning range of 1.3 × 1.3 mm^2, using lenses and deflection mirrors. PL from the sample was collected with an $F = 1.5$ lens system. The collected light was passed through narrow bandpass filters to extract a specific spectral component, and then transferred to the Ge detector.

3 Results and discussion

3.1 Microscopic and spectroscopic PL mapping

In Fig. 1, PL spectra at 300 and 4.2 K from the intra-grain defect region are shown. Deep-level emission with an intensity maximum at 0.78 eV was observed besides the band-edge (BE) emission at 300 K. Dislocation-related lines labeled D1–D4 appeared at 4.2 K together with the 1.09 eV line marked B_{TO} in the near band-edge region which is the TO-phonon replica of the boron bound exciton. We obtained the intensity mappings of respective spectral components extracted by the bandpass filters with a maximum transmission at 0.79, 0.81, 0.87, 0.93, 1.00 and 1.09 eV, as shown in Fig. 1. The intensity distributions of the 0.78 eV band and the BE emission at 300 K, and the D1, D2, D3, D4 lines and the B_{TO} emission at 15 K are shown in Fig. 1a–g, respectively. A loop-like dark-line defect was observed in the BE emission mapping at 300 K, as shown in Fig. 1b. The defect originates in the dislocation clusters which form small angle grain boundaries [3]. Several other dark-line patterns appeared besides the loop at 15 K (Fig. 1g). Figure 1c and d shows that the intensity of the D1/D2 lines was low at the loop and high in the nearby surrounding area. However, the intensity distributions of the D1 and D2 lines on and around the loop were complementary. The D3/D4 line mappings presented segmented patterns similar to the B_{TO} emission mapping at 15 K (Fig. 1e and f). We confirmed that the D-line patterns were grouped into two categories: D1/D2 and D3/D4 lines. This grouping also occurred for D-line mappings in dislocated single-crystalline silicon (sc-Si) [9]. The intensity of the 0.78 eV band was high at the core of the loop, as shown in Fig. 1a. These results clearly show that the origin of the 0.78 eV band is different from that of the D-lines.

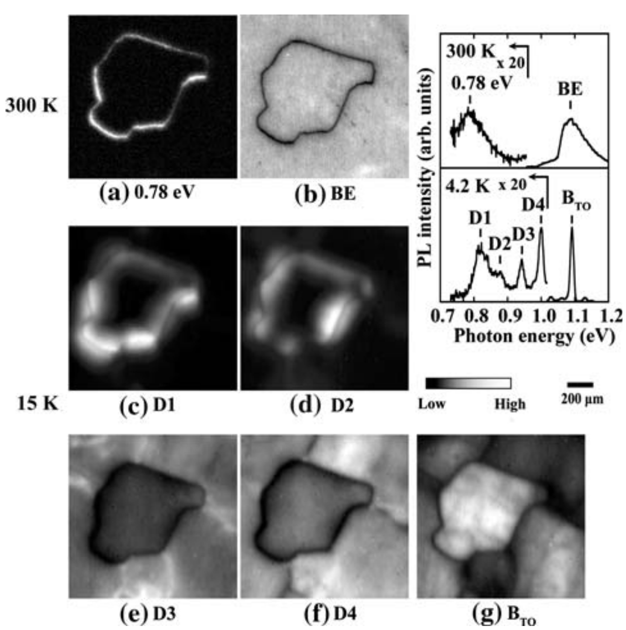

Fig. 1 Microscopic and spectroscopic PL mappings of (a) 0.78 eV band and (b) band-edge emission at 300 K, and (c) D1, (d) D2, (e) D3, (f) D4 and (g) B_{TO} emission at 15 K, respectively. Whiter gradation indicates higher intensity level. PL spectra at 300 K and 4.2 K from the mapped region are also shown

3.2 Temperature dependence of PL spectra

Figure 2 shows temperature dependence of PL spectra from the same area as Fig. 1. The intensity of the D-lines decreased with temperature and became less than our detection limit above 120 K. This result was similar to that of annealed Czochralski-grown silicon (CZ-Si) [10].

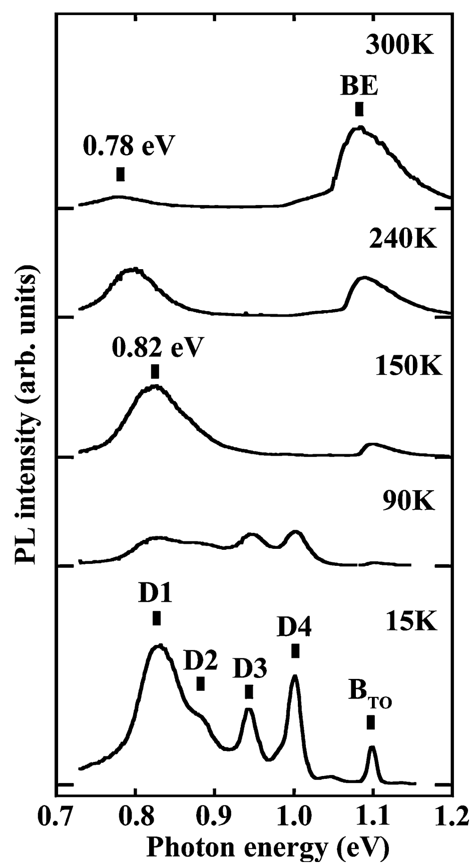

Fig. 2 Temperature dependence of PL spectra from intra-grain defect region in Fig. 1

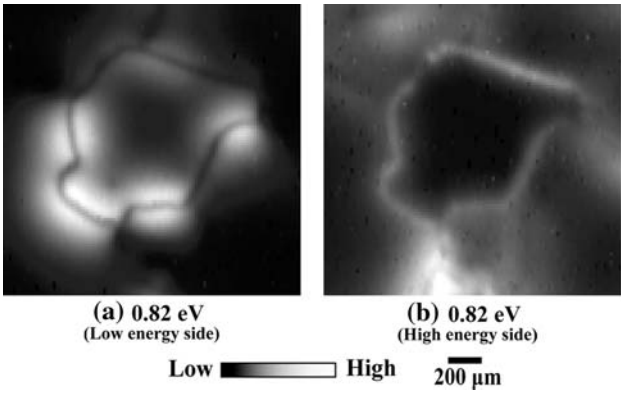

Fig. 3 Microscopic and spectroscopic PL mappings at 150 K of (**a**) low and (**b**) high energy side in the 0.82 eV band in the same area as Fig. 1

A broad band with a peak at 0.82 eV was observed at 150 K. The intensity of the 0.82 eV band increased with temperature, attained a maximum at 180 K, and then decreased with the peak shifting to the low energy side. The band remained as the 0.78 eV band at 300 K. We believe that the peak shift was due primarily to the band-gap shrinkage because this band shifted parallel to the position of the BE emission.

3.3 Origin of the 0.78 eV band

The intensity distributions of the low and high energy side in the 0.82 eV band are shown in Fig. 3a and b, respectively. The bandpass filters with a maximum transmission at 0.81 and 0.87 eV were used to monitor the respective emissions. The intensity distributions of the low and high energy side were different, which indicated the 0.82 eV band consisted of two components. The mapping pattern of the low energy side was the same as that of the D1 line, while that of the high energy side was similar to that of the 0.78 eV band. There has been discussion whether the 0.78 eV band and the D1 line have the same origin [4, 11] or not [5, 10]. The present results obviously show that the origin of the 0.78 eV band is different from that of the D1 line.

The results mentioned above were essentially the same as those of annealed CZ-Si [10]. We believe that the 0.78 eV band is the D_b band which is ascribable to oxygen precipitation [12]. Therefore, we conclude that the 0.78 eV band is associated with the oxygen precipitation, and that the intra-grain defects are dislocation clusters decorated with not only heavy-metal but also oxygen impurities.

4 Conclusions

We investigated the intensity distributions of the D-lines and the 0.78 eV band in the region including intra-grain defects, and studied the temperature dependence of the PL spectra. We confirmed that the origin of the 0.78 eV band is different from that of the D1 line. The present findings lead us to suggest that the 0.78 eV band is due to the oxygen precipitation, and that the intra-grain defects are dislocation clusters decorated with not only heavy-metal but also oxygen impurities.

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