Hyperfine Interact
DOI 10.1007/s10751-011-0450-1

Mapping analyses of Fe-diffused mc-Si using Mössbauer microscope and photoluminescence

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Abstract ^{57}Fe-diffused multi-crystalline silicon (mc-Si) wafer was studied by both Mössbauer and photoluminescence (PL) microscopes. By observing the ^{57}Fe doped and non-doped areas separated with grain boundaries, substitutional and interstitial Fe impurities appear to influence differently on the PL intensities, which are closely related to the carrier trappings at the Fe.

Keywords ^{57}Fe-mapping · Fe doped mc-Si · Mössbauer microscope · Photoluminescence

1 Introduction

Multi-crystalline silicon (mc-Si) wafers are widely used for solar cells whose energy conversion efficiency is about 16 to 17%. This value could be improved up to 25%, if one could remove metallic impurities as well as crystal defects from the wafers. The lattice defects have been investigated by different evaluation techniques for semiconductors. One of the most successful methods appears to be photoluminescence (PL) spectroscopy and its imaging technique [1, 2]. Silicon solar cells are known to contain Fe impurities with concentrations between 10^{11} Fe/cm^3 and 10^{17} Fe/cm^3 which originate from raw materials and also from the crucible used for melting and solidification processes. The metallic impurities form deep levels in the silicon band gap, leading to a strong degradation of the solar cells due to carrier trappings at the impurities.

In this study, we combined a PL mapping technique with a "Mössbauer microscope", the latter of which has been developed in our group [3–6], and investigated space correlations between Fe and lattice defects in an Fe-diffused mc-Si wafer.

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Table 1 Experimental conditions of Mössbauer-microscope and PL intensity mappings

	Mössbauer-microscope map	PL intensity map
Beam type	γ−ray	DPSS laser
Energy	14.4 keV	2.33 eV (532 nm)
Spot size	250 μm	20 μm
Mapping area	6×6 mm^2	2×2 mm^2
Division	40	160
Mapping step	150 μm	12.5 μm

2 Experimental procedure

A ^{57}Fe layer with a thickness of 1.7 nm was deposited on the surface of a p-type mc-Si wafer (10^{16} B/cm^3) using electron-beam evaporation through an Al mask. Then, the wafer was annealed at 1000°C for one week in a vacuum of 10^{-4} Pa and Mössbauer transmission spectra were measured at room temperature. The experimental details were described in our previous paper [4]. Subsequently, the ^{57}Fe-diffused mc-Si was evaluated over the same area by both the microscopic techniques. In the Mössbauer microscope, the 14.4 keV-γ-rays were focused down to 250 μm by a multi-capillary X-ray lens. The internal conversion and Auger electrons due to ^{57}Fe Mössbauer effect were measured as functions of X-Y coordinates of the sample surface by a micro-channel plate (MCP) detector. Furthermore, PL spectra were measured at room temperature by a micro-PL spectrometer (Photon Design, MPL-800-SRD) using the 532 nm line as an excitation source. The PL intensities were plotted as functions of X-Y coordinates to form a mapping image. Since the peak wavelength in a PL spectrum corresponds to the band-gap energy of silicon, the mapping image provides a distribution of lattice defects where the intensity would be much lower than that of a perfect Si crystal. The measurement conditions for both techniques are summarized in Table 1.

3 Results and discussion

Figure 1 shows mapping images of the ^{57}Fe-diffused mc-Si wafer observed by (a) Mössbauer microscope and (b) PL intensity mapping, respectively. The former image was overlapped on a picture obtained by field emission scanning electron microscope (FE-SEM) to compare the Fe distribution with the microstructure of the sample. The mapping intensity of the Mössbauer image depended on the numbers of ^{57}Fe which distribute differently in different crystal grains near the surface. On the other hand, the latter image appeared to depend on the regions of the sample, which were separated not only by the grain boundaries (pointed out by white arrows), but also by the edge of the Al-mask for Fe deposition (black arrows). Such different regions were surrounded with a white broken line. Figure 1c shows a schematic drawing containing the two typical areas: (i) ^{57}Fe deposited regions separated by the grain boundary (white arrow) and (ii) ^{57}Fe deposited and not deposited regions due to the edge of the Al-mask (black arrow). The two areas (i) and (ii) in Fig. 1c correspond to the broken square areas marked in Fig. 1a and b, respectively.

In the area (i), the Mössbauer mapping intensities were rather high in the upper left area, corresponding dominantly to substitutional Fe which distributed with a Gausian diffusion profile down to about 100 nm from the surface [5]. When crossing

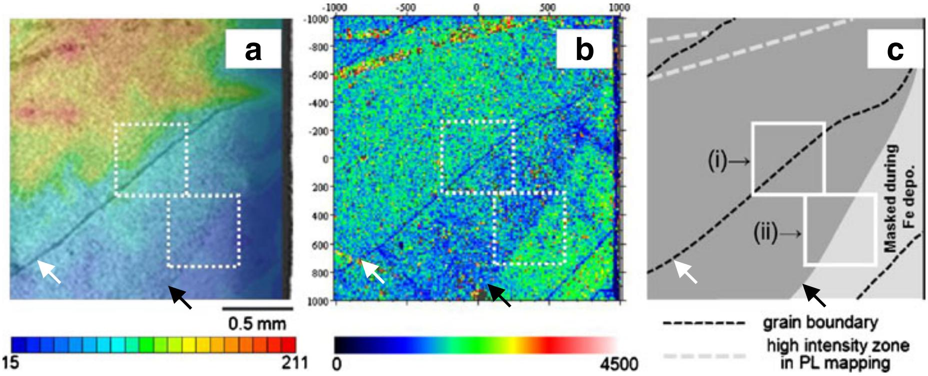

Fig. 1 2 × 2 mm^2-images observed in ^{57}Fe-diffused mc-Si: **a** composite of Mössbauer-microscope with FE-SEM, **b** PL intensity mapping, and **c** schematic drawing

the grain boundary from the upper left to the lower right region, the mapping intensity of substitutional Fe decreased abruptly at the boundary. On the other hand, relatively high PL intensities were found in the same region of the upper left, although this result apparently contradicted that observed by the Mössbauer microscope. A higer Fe concentration would lead to a lower PL intensity because of the carrier trappings at the Fe. However, substitutional Fe, which were distributing close to the surface, seem not to affect the PL intensity as strongly as in the case of interstitial Fe, the concentration of which was at least two orders of magnitude lower than that of substitutional Fe [5].

The area (ii) consisted of ^{57}Fe deposited and non-deposited regions at the upper left and the lower right of the square, respectively. The ^{57}Fe deposited region of the upper left showed a lower PL intensity, suggesting a considerable high concentration, although the Mössbauer intensity indicated a low Fe concentration. On the other hand, the PL intensity of the lower right region was considerably high, which was in accord with the fact that the region was masked during ^{57}Fe deposition. Generally, an Fe-doped Si contains interstitial Fe atoms distributing in the whole sample after the annealing at 1000°C. Accordingly, the PL intensity observed in the area (ii) reflect that interstitial Fe must exist in both the regions, but the concentrations of the interstitial Fe were different in these regions, yielding the low PL intensity in the upper left and the high intensity in the area (ii).

4 Summary

We have evaluated a ^{57}Fe-diffused mc-Si wafer by using both Mössbauer and PL microscopes. It was clear that the mapping intensities observed by the present investigations depend not only on the grain structure, but also on the Fe lattice sites and their distribution in the sample, which were produced during the annealing at 1000°C.

Acknowledgement This work was supported by a research grant from the Ministry of Education, Culture, Sports, Science &Technology in Japan for supporting strategic research projects of private university since 2010.

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