Stress analysis of multicrystalline Si with artificial grain boundaries to investigate the generation mechanism of dislocation clusters

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Macroscopic properties of multicrystalline materials are often controlled by the presence of crystal defects. In mutlicrystalline Si (mc-Si) for solar cells, dislocation clusters are known as the primary defects to act as recombination centers of photogenerated carriers and deteriorate the conversion efficiency. Therefore, it is essential to develop a crystal growth method to suppress the generation of dislocation clusters based on understanding their generation mechanism. However, the complicated crystal orientations and grain boundaries hamper the elucidation. We aim to elucidate the universal mechanism by combining macroscopic stress analysis, microscopic crystal structure analysis, and machine learning. In our previous study, we performed finite element stress analysis in a region where dislocation clusters were generated in mc-Si and found that macroscopic shear stress during crystal growth affects the propagation and growth of dislocation clusters [1]. In this study, we performed directional solidification using a seed crystal with artificial grain boundaries to permit systematic investigation for a variety of grain boundaries. We prepared 12 Si ingots containing artificial grain boundaries produced by the directional solidification method, and 48 artificial grain boundaries were investigated [2]. Two growth directions, <001> and <110>, were chosen. Fig. 1. is an example of a photoluminescence image of a 2 mm thick wafer cut parallel to the growth direction and perpendicular to the grain boundary, showing that the amount of dislocation generation differs for each grain boundary and grows with growth. The dislocation amount was defined as the percentage of the area where the brightness is lower than the threshold value on both sides of the grain boundary and was measured around 4 cm from the bottom. A three-dimensional temperature distribution was obtained based on crystal growth simulations to analyze the stress distribution in the Si ingot. The elastic modulus matrix was entered for each grain, and a finite element stress analysis was performed. Fig. 2. shows that the maximum shear stress for 12 slip systems from the analysis results, showing that the stress distribution is different for each grain, and that stress is concentrated at some grain boundaries. The red and blue dots in Fig. 3. show the results of grain boundaries with a growth direction of <001> and <110>, respectively. The results show that the grain boundary with <001> growth direction showed smaller dislocation generation and lower stress. These results suggest that dislocation generation could be suppressed by setting the growth direction to <001>. We will discuss the underlying mechanism on the impact of the growth direction on the generation of dislocations.

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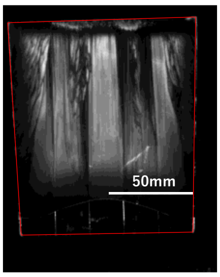

Fig. 1. Example of PL image of ingot

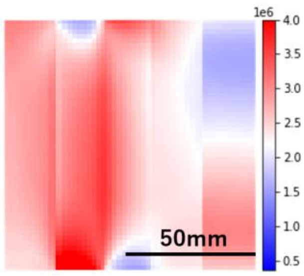

Fig. 2. Example of maximum shear stress distribution

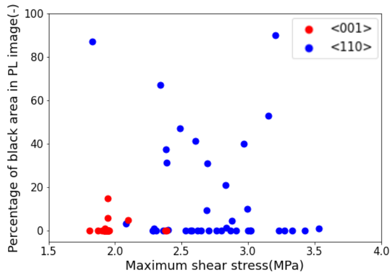

Fig. 3. Dislocation amount and maximum shear stress