Interaction of Grain Boundaries at Crystal/Melt Interface of Silicon

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What will happen when two grain boundaries meet at a crystal/melt interface? To answer this question, we directly observe the crystal/melt interface of multicrystalline silicon during directional solidification.

Multicrystalline silicon (mc-Si) grown through directional solidification is the dominant material in photovoltaic applications. A grain boundary (GB) in mc-Si is one of the most significant factors deteriorating the conversion efficiency of solar cells. However, the behaviors of GBs at a crystal/melt interface have not been well understood, especially with respect to the interaction between two GBs. Therefore, in this study, we have attempted to elucidate mechanisms behind GB interactions through *in-situ* observations during crystal growth.

Experiments were performed using an *in-situ* observation system consisting of a microscope and a crystallization furnace. The solidified silicon crystal samples were analyzed using electron backscattering diffraction (EBSD) to determine the grain orientations and structure of the GBs.

Figure 1 shows a crystal/melt interface of mc-Si during directional solidification, and Figure 2 shows the results of EBSD analysis of the observed area. Several grain boundaries, including small-angle grain boundary (SAGB) and Σ3 GB were observed in the growing crystal. A pair of straight {111}Σ3 GBs, confirmed by EBSD measurement (see Fig. 2(b-d)), grow slanting toward the lower-left region of the figure. This pair of {111}Σ3 GBs met another pair growing from the lower part (Fig. 1(4)). Fig. 2(c) shows the convergence of two pairs of {111}Σ3 GBs to produce a new Σ9 GB. This Σ9 GB later converged with a {111}Σ3 GB to form a new {111}Σ3 GB with a different growth direction, as shown in Fig. 2(c).

In contrast to this situation, Σ3 GBs did not interact with SAGBs during the solidification. From the *in-situ* observation snapshots shown in Fig. 1(3) and 1 (4), the SAGBs grew through the {111}Σ3 GBs without changing their direction of growth. This was confirmed by EBSD analysis, as shown in Fig. 2(d). The misorientation of SAGB did not change before and after the interactions with Σ3 GBs.

We also observed the interaction between two SAGBs, as shown in Fig. 2(e). $SAGB_1$ and $SAGB_2$ converge and only one GB with a slightly higher misorientation, referred to as $SAGB_3$, remains.

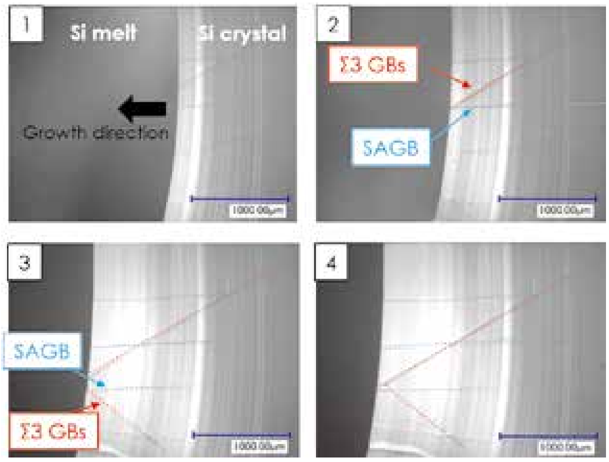

Fig. 1 Observation of interaction between GBs at crystal/melt interface in Si.

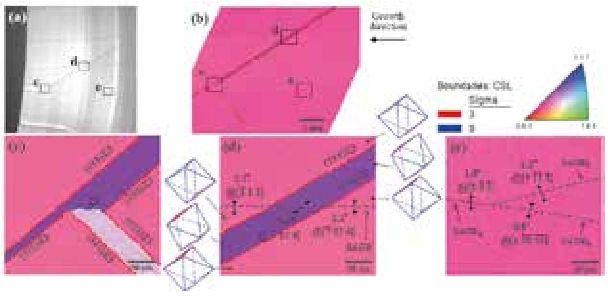

Fig. 2 EBSD analysis for characterization of observed GBs.

In this way, usually, when two GBs meet at a crystal/melt interface, a new GB is established (e.g., Σ3+Σ3→Σ9 and SAGB +SAGB→SAGB). However, interestingly, no such reaction occurs between SAGB and Σ3 GB, i.e., Σ3+SAGB→Σ3+SAGB, with no change of misorientation and direction.

References

[1] L-C. Chuang, K. Maeda, H. Morito, K. Shiga, W. Miller, and K. Fujiwara, Scr. Mater. **148**, 37 (2018).

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