

Impact of light element impurities on crystalline defect generation in silicon substrate

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1. Introduction

In order to improve the conversion efficiency of crystalline silicon solar cells, it is desired to reduce the crystalline imperfections, such as grain boundaries and defects. These imperfections act as minority carrier recombination center and degrade the conversion efficiency of solar cells [1]. On the other hand, although it is reported the chemical bonding of light element impurities, such as C, N, and O in multi-crystalline silicon substrate [2], the behavior of light element during crystalline growth is not well understood yet. We consider it is necessary to clarify the impurity effect on the crystalline growth to improve the crystal quality. In this study, we evaluated the impact of light element impurities on the generation of crystalline imperfections during the crystal growth. In order to control the interdiffusion of light element impurities, we regulated gas flow rate in the atmosphere. Additionally, seed crystal was used so that we could evaluate the impurity effect independently from those by grain boundaries.

2. Experiment

In the experiment, we fabricated B-doped silicon substrates by unidirectional solidification technique. We controlled the Ar gas flow in the atmosphere based on the computer simulation to reduce light element infusion in the Si melt during the crystal growth and compare with conventional one. We also used single crystal seeds for the growth. The sliced substrates were etched by HNO₃ and HF mixture to remove damaged surface layer. Then, the substrates were mechanically polished and chemically etched for the evaluation. We evaluated the crystalline defects in the single crystalline region at the center of ingot.

The substrates were etched by Secco etch mixture for 60 sec, then the etch pit densities were measured by SEM observation. The substrates were mechanically polished and chemically etched again for the detail evaluation of the defects. The defects and the misorientation angle at the small angle grain boundaries were evaluated by EBIC and EBSD, respectively. The structures of crystalline defects were also observed in detail by TEM.

3. Results and Discussion

The etch pit densities in the Si ingot formed by the conventional and controlled atmosphere were 1.5×10^5 - 7.0×10^7 and 5.0×10^3 - 4.0×10^5 cm⁻², respectively. In order to understand this significant difference in the defect densities by controlling Ar flow in the atmosphere, we evaluated defects distribution in the substrate with conventional Ar flow.

In the conventional sample, the etch pit density suddenly increased beyond a certain point, while the etch pit density increased moderately as crystalline growth procedure in the controlled sample. Figure 1 show the EBIC image where the etch pit density suddenly increased in the conventional sample. In this region, the contrasts in the EBIC image were precipitates consisted of C and N confirmed by SEM/EDX. The density of precipitates increased as crystalline growth procedure. Then, the small angle grain boundaries appeared in place of the precipitates as shown in Fig. 2 with EBIC image. The precipitations tended to occur at the small angle grain boundaries after their generation. Thus, we considered that small angle grain boundaries might be caused by the precipitations. Figure 3 shows TEM image taken at a precipitate. The line contrast extended from the precipitate is assigned as small angle grain boundaries, apparently consisting of dislocations. Slight misorientation and/or strain field were induced by the precipitates and they might generate the small angle grain boundaries as crystalline growth procedure.

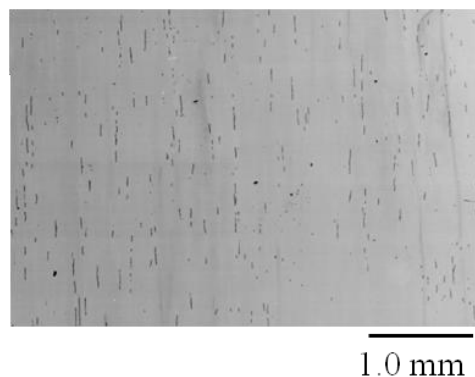


Fig. 1 EBIC image of precipitation in the conventional sample.

The etch pits and EBIC images at a small angle grain boundary in the conventional sample are shown in Fig. 4. In Fig. 4(a), it can be recognized that the etch pit densities were asymmetric across the boundary. In Fig. 4(b), the dark line is observed at the center, which was the small angle grain boundary defined by EBSD. Corresponding to the asymmetric etch pits, the EBIC image showed darker on the right side than the left side of the small angle grain boundary. The asymmetric defect densities across the small angle grain boundaries have been clearly explained by the asymmetric share stress introduction on both sides [3, 4]. This phenomenon implies the origin of the defects generation was the strain field. Thus, we considered the high density etch pits, which should express some small crystalline defects probably dislocations, were generated due to the strain field caused by the small angle grain boundary.

Therefore, in the crystal growth with light element impurities, the impurities precipitate first, and generate small angle grain boundaries, then the enhanced strain caused by the small angle grain boundaries resulted in the even higher density dislocations. Finally we concluded the cause of higher etch pit density in the conventional sample than that in the atmosphere controlled sample was light

element impurities introduced from atmosphere.

4. Conclusions

In conclusion, we confirmed the light element impurities can be an origin of the defect generation by comparing Si ingot grown in the conventional and controlled Ar flow in the atmosphere. The light element impurities precipitated first and the precipitates lead to the small angle grain boundary generation due to the slight misorientation and/or strain around the precipitates. Finally, the strain field caused by the small angle grain boundaries resulted in the high density small dislocations.

Acknowledgements

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References

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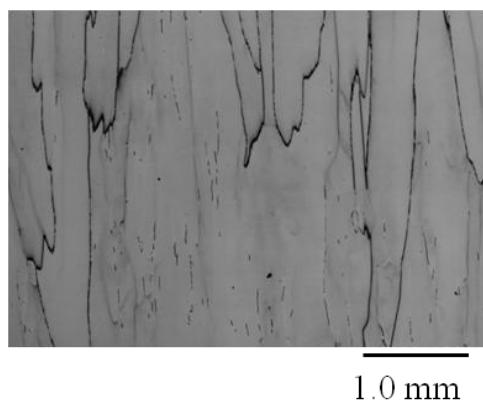


Fig. 2 EBIC image where the small angle grain boundaries appeared in place of precipitates.

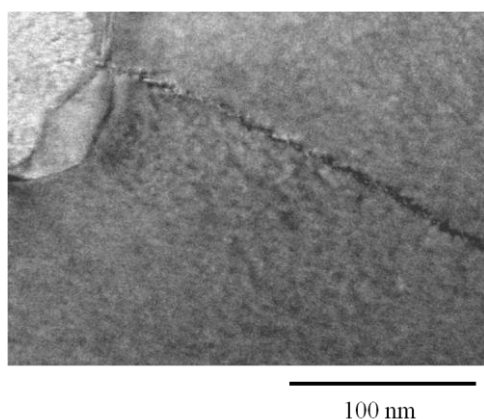


Fig. 3 TEM image at a precipitate.

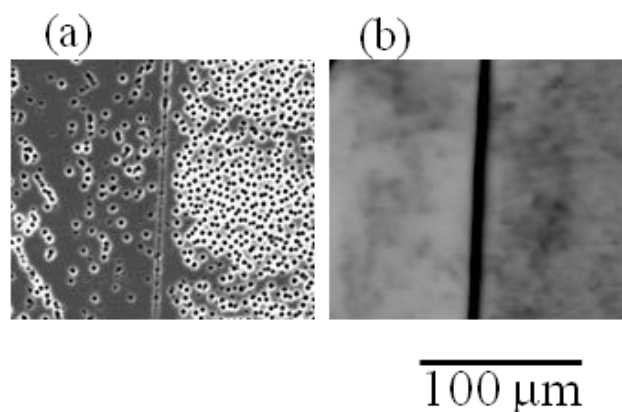


Fig. 4 (a) Etch pit and (b) EBIC images taken at asymmetric etch pit densities across a small angle grain boundary.