

Si 中の $\Sigma\{111\}/\{115\}$ 非対称粒界における双安定構造

Structural bistability in $\Sigma\{111\}/\{115\}$ asymmetric grain boundary in silicon

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Grain boundaries (GBs) are inevitably introduced in polycrystalline silicon (Si) ingots for solar cells, and they have substantial influences on electronic properties such as minority carrier lifetime, via the segregation of impurity atoms. Especially, asymmetric GBs with higher- Σ value of the associated coincident site lattice (CSL) are frequently introduced in Si ingots even though their GB energy is fairly high, and they severely affect the overall material properties even when their density is very low. Therefore, a comprehensive knowledge of the structural properties of the GBs, as well as the formation mechanism, is indispensable to produce cost-effective high-efficiency solar cells by controlling the formation of those detrimental GBs.

In the present study, we discuss the structural stability of asymmetric $\Sigma\{111\}/\{115\}$ GBs with the $\langle 110 \rangle$ tilt axis. In a cast-Si ingot, a GB has a periodic interface structure with a period of 2 nm along the GB, composed of 10 Si dumbbells which cannot be assigned to one of the two grains and 4 single-atomic columns with the stretched $\langle 110 \rangle$ reconstructed bonds [1]. The distorted dumbbells are oriented such that they form $\Sigma\{111\}$ -like nano-facets, suggesting a low GB energy in the range of the highly symmetric low- Σ GBs [1]. Actually, the GB energy is estimated to be about 0.45 J/m², and this is comparable to the GB energy of symmetric $\Sigma 9$ and $\Sigma 27$ GBs. Meanwhile, we have found a different interface structure with the similar period length in Czochralski (CZ)-grown Si ingots: one GB unit is composed of $\Sigma\{221\}$ -like and $\Sigma\{114\}$ -like nanofacets involving 2 single-atomic columns, revealed by high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) [2]. The latter GB unit can be formed by removing stacking faults on the $\Sigma\{111\}$ -like nano-facets in the former GB unit. Unlike in the former GB unit, the HAADF signal of the atomic columns do not drop in the latter GB unit, indicating that the latter GB unit would not involve partial site occupancies and static atomic displacements. Even though the small number of the stretched $\langle 110 \rangle$ reconstructed bonds and small atomic strains, the GB energy of the latter GB unit, estimated to be 0.6 J/m², is slightly higher than that of the former GB unit. The formation process of those bistable asymmetric GB structures will be discussed.

[1] A. Stoffers, *et al.*, Phys. Rev. Lett. 115 (2015) 235502.

[2] Y. Ohno, *et al.*, Appl. Phys. Lett. 110 (2017) 062105.

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