Σ3{111}対称傾角粒界の不純物偏析能とキャリア再結合速度に対する傾角のずれの影響

Impact of the deviation of the tilt angle on the recombination activity and the impurity segregation ability of Σ3{111} symmetric tilt boundaries

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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 carrier recombination activity, 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, and they severely affect the overall material properties even when their density is very low. Therefore, a comprehensive knowledge of the recombination activity of the GBs, as well as their impurity segregation ability depending on their atomistic structure, is indispensable to produce cost-effective high-efficiency solar cells by controlling the formation of detrimental GBs.

In the present study, we discuss the recombination activity of asymmetric Σ3{111} GBs with the <110> tilt axis, whose GB planes are slightly inclined from {111}. Even though the activity is negligible for the symmetric Σ3{111} GBs of which the GB plane is just on {111} [1], the activity is high for the asymmetric ∑3{111} GBs even when their inclination angle is small. High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) reveals that, most segments of the asymmetric GBs are composed of arrays of GB dislocations lying on symmetric Σ3{111} GBs. Those dislocations are edge-type with the Burgers vector of 1/3<111>. Atom probe tomography (APT) reveals that oxygen atoms would segregate at the atomic sites under tensile stress above about 2 GPa, which are introduced along the GB plane due to the GB dislocations [2-4]. Carbon atoms also segregate, while they would locate only nearby the dislocation cores. The correlation between the recombination activity and the segregation ability of impurity atoms will be discussed.

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