シリコン中の傾角粒界における酸素の偏析機構

Segregation mechanism of oxygen atoms at tilt boundaries in silicon

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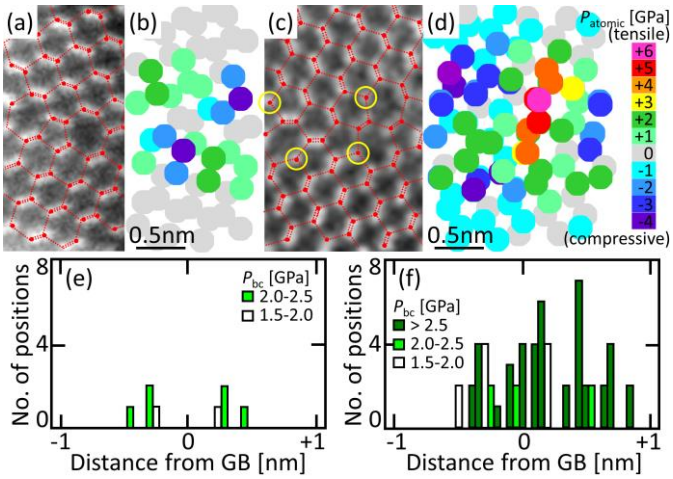
Grain boundaries (GBs) in Czochralski- (CZ-) and cast-grown Si ingots used for solar cells have serious impacts on the solar cell efficiency via the segregation of detrimental impurity atoms, such as oxygen and transition metals introduced inevitably during crystal growth and cell processing, depending on their structural condition at those GBs. Accordingly, precise understanding of the segregation mechanism of impurity atoms is one important issue to produce cost-effective solar cells by engineering the structural condition of impurity atoms segregating at GBs.

In this work, 3D distribution of oxygen atoms segregating at the typical large-angle GBs (Σ3{111}, Σ9{221}, Σ9{114}, Σ9{111}/{115}, and Σ27{552} GBs) in Cz-grown Si were systematically determined by atom probe tomography with a low impurity detection limit (0.005 at.% on a GB plane) simultaneously with a high spatial resolution (about 0.4 nm), and it was correlated with the atomic stresses around the GBs estimated by ab-initio calculations based on the data of atomic-resolution transmission electron microscopy. The high resolution analyses revealed that oxygen atoms preferentially segregated at the bond-centered positions under tensile stresses above about 2 GPa, so as to attain more stable bonding network by reducing the local stresses. The number of segregating atoms per unit GB area (N_{GB}) was estimated as a function of the number of the tensilely-stressed positions per unit GB area (n_{bc}) and the average concentration of oxygen atoms around the GB ([O_i]): $N_{GB} \sim 50 n_{bc}[O_i]$. This atomistic segregation mechanism at GBs would provide a guidance to optimize the solar cell efficiency by engineering the distribution of oxygen atoms at the GBs in controlled fashions, as well as by controlling metallic contaminants via gettering and/or annealing processes disturbed by oxygen precipitates, and it will lead to producing cost-effective high-efficiency solar cells.



(a, c) Bonding network and (b, d) distribution of atomic stress P_{atomic} at (a, b) Σ9{221} and (c, d) Σ9{114} GBs in Si. Number of bond-centered positions under a tensile stress P_{bc} above 1.5 GPa for (e) Σ9{221} and (f) Σ9{114} GBs.