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## Chemical nanoanalyses of Si grain boundaries towards the fabrication of high- functional Si solar cells

Polycrystalline materials with grain boundaries (GBs), involving excess free energy because of their structural imperfection, can reduce their energy by the nanoscopic structural changes of the GBs via impurity segregation. Those local changes at GBs can stabilize non-equilibrium nanostructures, resulting in the drastic change in the macroscopic properties of those materials. The mechanism of GB segregation is, however, far from being understood due to difficulties in characterizing both crystallographic and chemical properties of the same GB at atomistic levels. We have therefore developed an analytical method to determine the impurity segregation ability on the same GB at the same nanoscopic location by a joint use of atom probe tomography (APT) and scanning transmission electron microscopy (STEM) combined with *ab initio* calculations, and discussed the segregation mechanism at atomistic levels. Three-dimensional distribution of impurity atoms was systematically determined at the typical large-angle GBs, small-angle GBs, and dislocations on GBs in Si by APT with a high spatial resolution (about 0.4nm), and it was correlated with the atomic stresses around the GBs estimated by *ab initio* calculations based on atomic-resolution STEM data. It was shown that impurity atoms preferentially segregated at the atomic positions under specific stresses so as to attain a more stable bonding network by reducing the local stresses. For example, the number of segregating oxygen atoms per unit GB area ($N_{GB}$) is proportional to both the number of the stressed positions per unit GB area ($n_{bc}$) and the average concentration of oxygen atoms around the GB ($[O_i]$) with $N_{GB} \sim 50 n_{bc}[O_i]$.

### Biography

Yutaka Ohno (PhD: Physics) is working in the Institute for Materials Research, Tohoku University (http://www-lab.imr.tohoku.ac.jp/~yutakaohno/). He is also working in the CREST research project (Grant No. JPMJCR17J1 (2017-2023)) in Japan Science and Technology Agency. A focus is on quantitative analyses of the impurity segregation ability of grain boundaries in Si and compounds by atom probe tomography (APT, with a spatial resolution less than 0.4nm) combined with scanning transmission electron microscopy (STEM) and *ab initio* calculations, but also on the study of atomistic structures of semiconductor nanostructures by optical measurements (cathodoluminescence, micro-photoluminescence, near-field optical measurements) under TEM.

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