シリコン中の大角粒界における不純物の偏析能

Segregation ability of impurity atoms at large-angle grain boundaries in Si

IMR, Tohoku Univ.[1], The Oarai Center, IMR, Tohoku Univ.[2], ISIR, Osaka Univ.[3], AIST[4],

°Yutaka Ohno[1], Kaihei Inoue[1], Kozo Fujiwara[1], Kentaro Kutsukake[1], Momoko Deura[1], Ichiro Yonenaga[1], Yasuo Shimizu[2], Koji Inoue[2], Naoki Ebisawa[2], Yasuyoshi Nagai[2], Hideto Yoshida[3], Seiji Takeda[3], Shingo Tanaka[4], Masanori Kohyama[4]

E-mail: yutakaohno@imr.tohoku.ac.jp

Grain boundaries (GBs) in multicrystalline silicon (m-Si) can act as preferential segregation sites for impurity atoms. The segregation ability depends on the GB character, and the structure, size and distribution of impurity agglomerates at GBs determine the electronic properties. Accordingly, it is important to control the impurity conditions at GBs for the production of m-Si based functional devices. The segregation mechanism is, however, far from being understood due to difficulties characterizing both crystallographic and chemical properties of the same GBs at an atomistic level.

In the present work, we examined three-dimensional (3D) distribution of light impurity atoms (O and C) (Fig. 1a), as well as dopant atoms (Ga, As, B), at the typical large-angle GBs in m-Si by atom probe tomography (APT) with a high spatial resolution (about 0.4 nm) simultaneously with a low impurity detection limit (0.005 at.%). The intrinsic segregation abilities for the GBs were assessed, and they were discussed in terms of bond distortions at the GBs revealed by ab-initio calculations based on the experimental results of scanning transmission electron microscopy (STEM) (Fig. 1b). Bond distortions inducing atomic stresses were intrinsically inherent around the GBs. The concentration profiles across the GBs for each kind of impurity atoms were correlated with the distribution of the atomic sites under a specific atomic stress. It is hypothesized that, an impurity atom can segregate at an atomic site whose atomic stress is reduced by the impurity atom, and the segregation ability increases with increasing the stress reduction as a result of the impurity segregation. The segregation ability, therefore, depend both on the site stress and on the site density, and increases with increasing the GB energy (Figs. 1c and 1d).

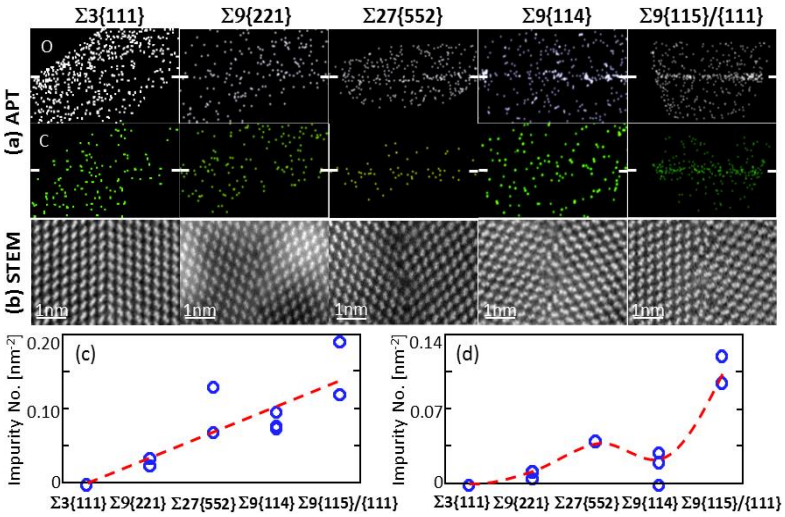

Fig. 1 (a) Projected 3D distribution of O and C atoms at the typical large-angle GBs shown in (b). Number of segregating impurity atoms per unit GB area; for (c) O and (d) C atoms.