シリコン中のヒ素ドーパントの粒界偏析機構

Mechanism for segregation of arsenic dopants at grain boundaries in silicon

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Arsenic (As) atoms, as important *n*-type dopants in silicon (Si), are frequently used for Si nano-devices due to their excellent properties, such as high solubility (1.8×10^{21} cm^{-3}) needed for low resistivity and low diffusivity (about 1/10 in comparison with the other important *n*-type dopants of phosphorus atoms) used for diffused junctions and buried layers that can resist annealing processes. Meanwhile, they can diffuse in GBs with a diffusivity four orders of magnitude higher than the single-crystal value, and therefore they preferentially segregate at GBs, rather than distribute homogeneously in grains, inducing undesirable inhomogeneous dopant distribution. In order to determine the segregation mechanism, three-dimensional distribution of As atoms at Σ3{111}, Σ9{221}, Σ9{114}, Σ9{111}/{115}, and Σ27{552} GBs is examined by atom probe tomography (APT) combined with low-temperature focused ion beam (LT-FIB), scanning transmission electron microscopy, and *ab initio* calculations. It is shown that,

1) Σ3{111} GBs, of which the GB energy is negligible, do not exhibit As segregation since they have little bond distortion and no dangling bond inducing deep levels.
2) As atoms segregate at Σ9{221} and Σ27{552} GBs in which no defect level exists while bond distortions exist, and the segregation ability increases linearly with increasing the GB energy. *Ab initio* calculations suggest that As atoms would locate at the GB sites under tensile stresses via elastic interactions, similar to the oxygen segregation in which the local bond distortions are reduced so as to attain a more stable bonding network [1].
3) The segregation ability for Σ9{114} or Σ9{111}/{115} GBs is much higher than the ability expected from the above elastic-interactions model. APT combined with LT-FIB suggests preferential As segregation at <1-10> reconstructed bonds under high tensile stresses. It is hypothesized that As atoms preferentially form As dimers at the reconstructed bonds, due to the tendency of As with five valence electrons to form a three-coordinated configuration so as to accommodate an excess electron in the dangling bond, which is efficiently attained by an As dimer. Since the reconstructed bonds would be introduced in the <1-10> tilt GBs with the tilt angle larger than 70.5° [2], the segregation ability of the GBs would be enhanced via the electronic effect.

As a result, our work provides important insights on As segregation at GBs in Si; it is determined not only by elastic interactions due to the intrinsic lattice distortions at GBs, but also by electronic interactions depending on the characteristics of valence electrons of As atoms as well as on local atomic configuration at GBs.

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