Interaction energy of dopant atoms with stacking faults in Si

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Grain boundaries and crystal interfaces including stacking faults are a key issue for high performance photovoltaic and/or electronic devices fabricated with Si crystals. It is theoretically expected that a stacking fault interacts with point defects such as dopant atoms, and the interaction would modify the electronic and mechanical properties in Si with stacking faults. In the present work, we have determined the segregation of various kinds of dopant atoms nearby stacking faults, by means of transmission electron microscopy and ab-initio calculations, and evaluated the interaction energy.

In Si crystals, the width of a stacking fault ribbon bound by a pair of partial dislocations increased when n-type dopant atoms (P, As, and Sb) segregated nearby the ribbon [1-3], while the width was unchanged when p-type dopant atoms (B and Ga) segregated [2, 4]. The origin of the increase for n-type dopant atoms was explained as the reduction of the stacking fault energy due to an electronic interaction between the ribbon and the dopant atoms segregated at the ribbon, rather than as the reduction of the strain energy around the partial dislocations due to the dopant atoms segregated nearby the partials [3]. Actually, ab-initio calculations indicated that, P atoms would segregate at a stacking fault under an electronic interaction and the segregation results in the reduction of the stacking fault energy, while B atoms would not interact with stacking faults [4]. The interaction energy was estimated to be 0.15±0.05 eV by using a simple model based on the segregation probability of dopant atoms at a stacking fault [4], on the analogy of the segregation at a dislocation [5].

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