Electronic structure of dopant around stacking fault in Si crystal

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Dislocation cores of heavily doped n- and p-type Si crystals have been observed via transmission electron microscopy (TEM) by Ohno *et al.*[1]. When an n-type dopant (P, As, or Sb) is added, the dissociation width of stacking faults increases with increasing annealing time. Because the dissociation width of the stacking fault is determined by the balance between the stacking fault energy and repulsion of the dislocation cores, an increase in the stacking fault width indicates a decrease in stacking fault energy.

To investigate the experimental results of the segregation of dopant atoms around the stacking fault, we performed an energy assessment using Vienna ab initio simulation package (VASP). Our results indicate that both p-type (P, As, Sb) and n-type (Al, Ga, In) dopant atoms reduce the stacking fault energy when these atoms localize around the stacking fault.

To describe the dopant behavior in the stacking fault region in Si crystal, we proposed a new model as illustrated in Fig.1[2]. When the n-type dopant atoms are substituted at the stacking fault region (SF), the donor levels and total energy are shifted to lower energies. Conversely, when the p-type dopant atoms are substituted at the stacking fault, the system is unaffected by the change in the acceptor level because of the acceptor level do not contain any electrons, whereas the valence band shifts to lower energies and reduces the total energy.

[1] Y. Ohno *et al.*, Appl. Phys. Lett., **95** (2009) 091915.

[2] Y. Yamamoto *et al.*, Jpn J. of App. Phys., **53** (2014) 061302.

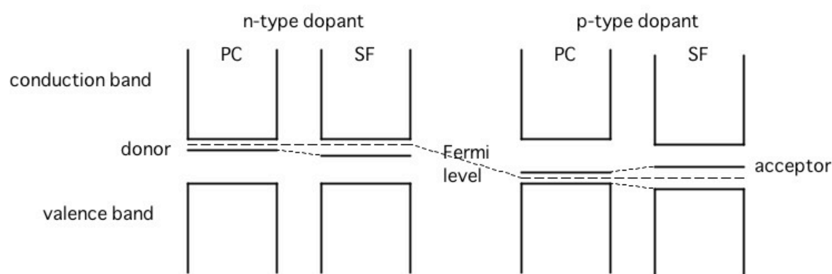

Fig.1 Schematic illustrations of the electronic structure changes for describing the n- and p- type dopant behavior around stacking faults in Si crystal.