Theoretical Study of the Stability of $X@B_6$ and $X@B_{12}$ Clusters: X=H–Br in Crystalline Silicon

Yoshitsune HIGASHIGUCHI, Hiroaki OCHIAI, Kazuyuki IGEI, Kengo OHMORI, and Yoshinoro HAYAFUJI

Ab initio calculations of the atomic and electronic structure of crystalline silicon (c-Si) with $X@B_6$ and $X@B_{12}$ (X=H-Br) clusters have been performed to investigate carrier generation by doping atoms inside the cage of the boron clusters. We confirmed that octahedral B_6, cubo-octahedral B_{12} (B_{12}-CO) and icosahedral B_{12} (B_{12}-ICO) can exist stably in c-Si and should act as double acceptors. We also found that H atoms can be settled in B_{12}-CO clusters and the $H@B_{12}$-CO cluster can introduce a very shallow single acceptor level whose activation energy is lower than those of B_6, B_{12}(-CO, -ICO) and substitutional boron atom (B_s). It is found on the basis of the formation energies that $B@B_6$ and $B@B_{12}$ will inevitably be formed and may degrade the efficiency of carrier generation. The $H@B_{12}$-CO cluster is one of the most promising candidates as the cluster dopant for the improvement of the efficiency of boron implantation and the formation of a high-performance extremely shallow junction.