Theoretical Study of the Stability of X@B_{6} and X@B_{12} Clusters: X=H–Br in Crystalline Silicon

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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.