Boron Clusters in High-Dose Implanted Silicon

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The electronic structures and X-ray photoelectron spectra of silicon models with octahedral B$_6$, icosahedral B$_{12}$, or cubo-octahedral B$_{12}$ clusters are investigated using first-principles calculations. It is found that the B$_{16}$ and B$_{12}$ clusters acts as double acceptors in silicon and that the simulated chemical shift of the B 1s orbital signals of the B$_6$ and cubo-octahedral B$_{12}$ clusters in X-ray photoelectron spectra coincides exactly with the chemical shift of B 1s experimentally observed in as-implanted silicon at an extremely high dose of boron. These results reveal that B$_6$ and cubo-octahedral B$_{12}$ clusters are the origin of hole carries in silicon. We propose a mechanism for hole generation and a physical model for boron cluster formation at implantation-induced divacancy sites and multi vacancy sites.