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 cubooctahedral 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 snd that the simulated chemical shifty of the B 1s orbital signals of the B_6 nad 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.