CALCULATIONS OF CHARACTERISTICS OF IMPURITY-DEFECT COMPLEXES IN SILICON AT HIGH CONCENTRATIONS OF IMPURITIES

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Summary

Microscopic mechanisms of an influence of point defect — impurity complexes on atomic rearrangements in a silicon crystal which is saturated by defects are theoretically investigated. To achieve the goal, a model that describes the silicon crystals with concentrations of defects more than 10^{21} cm^{-3} has been developed. For the model crystal, electronic structure and energetic characteristics are calculated by the electron density functional method and the first-principle pseudopotentials. Maps of the electron density distribution as well as potential reliefs for a displacement of impurity atoms (boron, phosphorus) are obtained. It is shown that, at critical concentrations of P_s and B_s, $(P_s)_2$ and $(B_s)_2$ complexes appear which turn into $P_iV_2P_i$ and $B_iV_2B_i$ complexes in a non-activation manner and serve as the generators of divacancies.