SI DOPING OF BETA-GA2O3 DEFECT CALCULATION

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Calculation of the band structure and other properties in β-Ga2O3 for Si implanted in the crystal instead of GaI, GaII was performed by the density functional theory method in the plane-wave basis (projector augmented wave - PAW) using Ga pseudopotentials, taking into account 3d valence electrons. The expansion in the plane-wave basis was carried out up to an energy of 520 eV. The hybrid exchange-correlation functional Heyd-Scuseria-Ernzerhof HSE [1] with mixing parameters α=0.35, µ=0.20 Å-1 was used for the calculation. To calculate the thermal stability of implanted defects, the Nudged Elastic Band method was used from first principles. Several nonequivalent positions of defects in the β-Ga2O3 lattice were considered. Defects were considered at concentrations of 5, 10, 15.20% by weight

Changes in the width and topography of the band structure and the mobility of charge carriers are obtained.

ЛИТЕРАТУРА

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