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Mutual Passivation of Donors and Isovalent Nitrogen in GaAs
JINGBO LI, PIERRE CARRIER, SU-HUAI WEI, National Renewable Energy Laboratory, SHU-SHEN LI, JIAN-BAI XIA, State Key Lab for Superlattices and Microstructures, Institute of Semiconductors, CAS — Using large supercell total energy and band structure calculations, we have studied the mutual passivation mechanism of isovalent N and shallow donors in GaAs. We find that all the donor impurities, Si_{Ga}, Ge_{Ga}, S_{As}, and Se_{As}, bind to N in GaAs:N, which has a large N-induced band gap reduction relative to GaAs. For group-IV impurity such as Si, the formation of the nearest-neighbor Si_{Ga}-N_{As} defect complex creates a deep donor level below the conduction band minimum (CBM). The coupling between this defect level with the CBM pushes the CBM upwards, thus restoring the GaAs band gap; the lowering of the defect level relative to the isolated Si_{Ga} shallow donor level is responsible for the increased electrical resistivity. Therefore, Si and N mutually passivate each other's electrical and optical activities in GaAs. For group-VI shallow donors such as S, the Coulomb binding between S_{As} and N_{As} does not form a direct bond and a deep level inside the gap; thus, no mutual passivation exists in the GaAs:(S+N) system. We also explained the difference between the mutal passivation of Si and N and the mutal passivation of H and N in GaAs. Our study provides a deep understanding of the mutual passivation mechanism and explained some of the recent puzzling experimental observations.

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