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Hybrid functional studies of stability and diffusion of hydrogen in Mg-doped GaN JI-SANG PARK, K.J. CHANG, Department of Physics, Korea Advanced Institute of Science and Technology — Nitride semiconductors are known to suffer from low p-type doping efficiency due to the high activation energy of Mg acceptors and the compensation of hole carriers. To enhance hole carrier concentration, the hydrogen co-doping method is widely used, in which hydrogen is intentionally doped with Mg dopants and removed by subsequent thermal annealing. In this work, we perform first-principles density functional calculations to study the stability and diffusion of hydrogen in Mg-doped GaN. For the exchange-correlation potential, we employ both the generalized gradient approximation (GGA) proposed by Perdew, Burke, and Ernzerhof and the hybrid density functional of Heyd, Scuseria, and Ernzerhof. We examine the diffusion pathways and dissociation barriers of H from the Mg-H complex using the nudged elastic band and dimer methods. We compare the results of the GGA and hybrid density functional calculations for the stability of various H interstitial configurations and the migration barriers for H diffusion. Finally, using the calculated migration barriers as inputs, we perform kinetic Monte Carlo simulations for the dissociation of the Mg-H complex and find that the Mg acceptors are activated by thermal annealing up to 700-800 °C, in good agreement with experiments.

Ji-Sang Park
Dept of Physics, Korea Advanced Institute of Science and Technology

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