MAR06-2005-000068

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

Interaction of the N vacancy with H and Mg acceptors in p-type GaN[1]

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Results from recent experimental studies suggest that the N vacancy (V_N) may compensate Mg acceptors in GaN in addition to the compensation arising from H introduced during growth. To investigate this possibility further, density-functional-theory calculations were performed to determine the interactions of V_N with H, Mg, and the MgH center in GaN, and modeling was performed to determine the state populations at elevated temperatures. The results indicate that V_NH and MgV_NH complexes with H inside the vacancy are highly stable in p-type GaN and act to compensate or passivate Mg acceptors. Furthermore, barriers for formation of these complexes were investigated and the results indicate that they can readily form at temperatures $> 400^\circ$ C, which is well below temperatures typically used for GaN growth. Overall, the results indicate that the V_N compensation behavior suggested by experiments arises not from isolated V_N, but rather from V_NH and MgV_NH complexes with H located inside the vacancy.

[1]Supported by the Office of Basic Energy Sciences, US DOE. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the US DOE under Contract DE-AC04-94AL85000.

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