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Interaction of hydrogen with defects in GaN YEVGENIY PUZYREV, MATTHEW BECK, Vanderbilt University, BLAIR TUTTLE, Penn State Erie, RON SCHRIMPF, DAN FLEETWOOD, SOKRATES PANTELIDES, Vanderbilt University — Hydrogen has long been known to have a dual role in Si electronics. It can passivate interfacial dangling bonds and other defects, but it can also be an agent of degradation and aging because it can be released under a variety of conditions. When released, it can depassivate other defects by forming H_2. In GaN, H has been known to play a key role in p-type doping (it helps Mg enter substitutionally, with an H attached to it; H is then removed to activate the Mg as a dopant). Here we present results of first-principles density-functional calculations exploring the role of H as a degradation agent in GaN devices, e.g., degradation by hot electrons. We find that H binds strongly to N antisite defects and is not removed during the process of dopant activation. Under normal operating conditions, hydrogenated N antisite defects are benign. However, hot electrons can release the H atoms from these defects, making them active electron traps. The results provide an explanation of pertinent data on hot-electron device degradation. This work was supported in part by an AFOSR MURI grant.

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