The Interaction of Defects and H in Proton-irradiated GaN(Mg,H)

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Motivation—P-type GaN is an increasingly important material because it is the hole-injecting layer in a variety of GaN and AlGaN-based light-emitting diodes (LEDs). The interactions of grown-in hydrogen with magnesium acceptors and the self compensation of acceptors by native defects are both important issues which must be understood before the full potential of this semiconductor can be realized. Local vibrational modes (LVMs), visible with fourier transform infrared spectroscopy (FTIR), can be studied to learn more about native defects that are otherwise difficult to probe.

Accomplishment—In order to study defects whose low equilibrium densities make detection difficult, magnesium-doped, p-type GaN containing H was irradiated with MeV protons at room temperature and then annealed at a succession of increasing temperatures, with the behavior of defects and H in the material being followed through infrared absorption spectroscopy, nuclear-reaction analysis (NRA) of the H, and photoluminescence. In the as-grown condition H from the MOCVD growth environment complexes with Mg acceptors, creating a distinctive LVM at 3122 cm^{-1} (Fig.1). The isotopic variant of this same mode at 2319 cm^{-1} is visible when hydrogen is removed from the material with a 900°C anneal and replaced with deuterium (Fig. 2). After implantation with protons which are energetic enough to pass all the way through the GaN film, the LVM spectra evolve as both as-grown and deuterium exchanged samples are heated in a sequence of one-hour vacuum anneals (Figs. 1 and 2). Beginning at 300°C the MgH(D) LVM is replaced with new H and D-related modes at 3134 and 2328 cm^{-1}. At annealing temperatures of 500°C and above these new modes begin to disappear and the original MgH(D) LVM is partially restored. Finally, above 700°C, all LVMs disappear, and at 800°C NRA data indicate that H(D) has left the material completely. Figure 3 shows the temperature dependence of the MgD mode and the "new mode" at 2328 cm^{-1}. It also shows the evolution of a new green luminescence peak which is only seen in these proton-irradiated and thermally annealed samples. Because theoretical studies indicate that Ga interstitials should be highly mobile at room temperature, we believe that Ga interstitial-vacancy Frenkel pairs should anneal out after the 300°C thermal treatment. This leaves N vacancies and interstitials as the defects which are most likely to produce the effects seen in Figs. 1-3. Because the frequency differences between the MgH(D) LVMs and the new modes are small, it is likely that the atomic configurations of the new defects are only slightly different from the known arrangement of the MgH(D) complex. This is consistent with the movement of an N interstitial to a site adjacent to the original complex. The complete disappearance of all H(D) related modes (Fig. 3) well before H has left the material suggests that H can find another trap in the GaN. Theory suggests that this "LVM-invisible" trap is the N vacancy, since its predicted LVM should be at wavelengths where the GaN substrate is strongly absorbing.

Significance—This work identifies a new native-defect-related structure in GaN. It has also provided insights into possible H trapping in GaN which has N vacancies introduced during the film growth process. Other Sandia research has also shown evidence for this effect.

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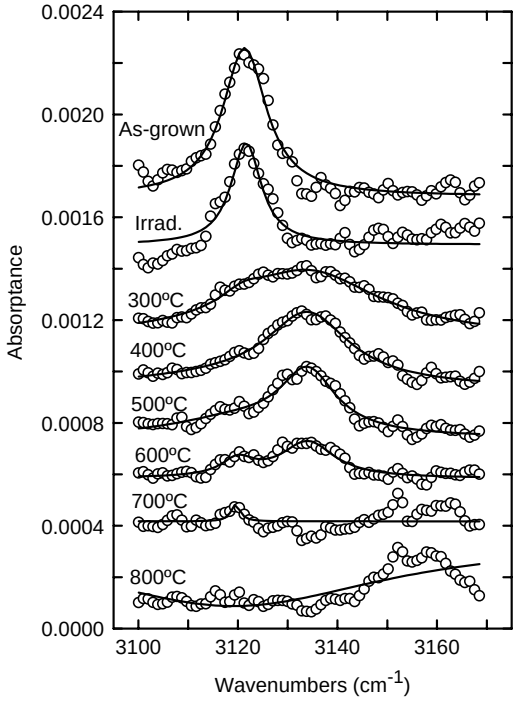

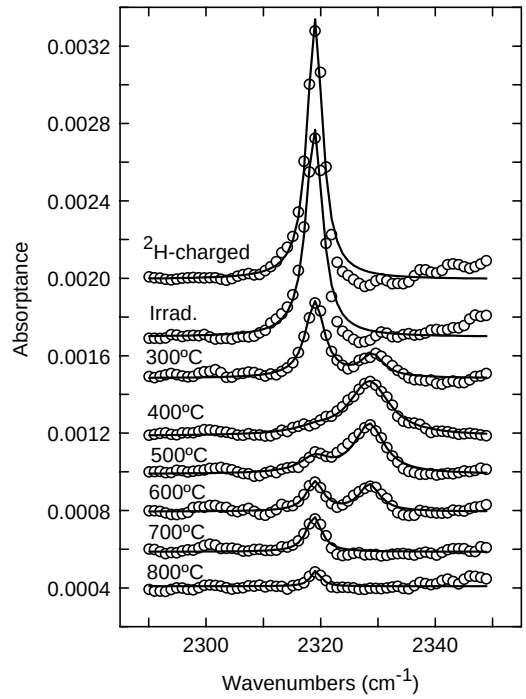

Figure 1 (left) and **Figure 2** (right). Sequential IR absorption spectra from specimens containing grown-in ^{1}H (Fig. 1) or ^{2}H exchanged for ^{1}H after growth (Fig. 2). The samples were irradiated at room temperature with 1-MeV protons and then subjected to a series of 1-hour vacuum anneals. The irradiation dose was 1.65×10^{16} cm^{-2}. The curves represent Lorentzian fits used to evaluate absorption strengths.

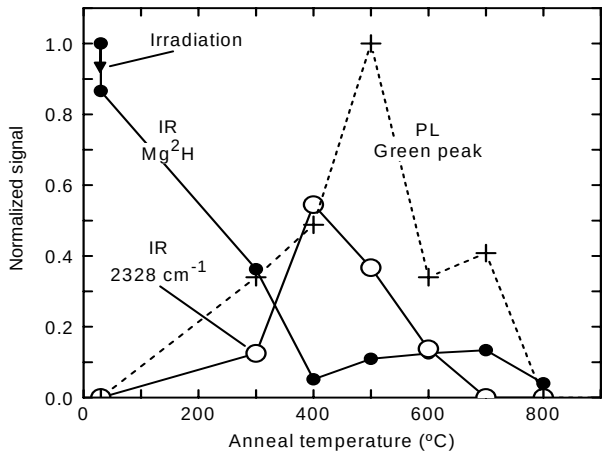

Figure 3. Normalized amplitudes of the IR absorption and green photoluminescence versus anneal temperature for a ^{2}H-charged specimen that was irradiated and then vacuum annealed.