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Influence of Fermi-level on the lattice location of 27Mg in GaN

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During 2017 we focused on investigating the lattice location of 27Mg as a detailed function of implantation temperature, implanted fluence, and fluence rate in different doping types of GaN: undoped GaN, as well as Si-doped n-type, Mg-doped p-type, and Mg-doped as grown.

The amphoteric nature of Mg, i.e. the simultaneous occupation of substitutional Ga and interstitial sites previously reported [1], was fully confirmed: following ultra-low fluence ('2E10 cm-2) room temperature (RT) implantation, the interstitial fraction of Mg was highest (20-25%) in the two samples that were pre-doped with 2E19 cm-3 stable Mg during epilayer growth, and lowest ("8%) in Si-doped n-GaN, while undoped GaN showed an intermediate interstitial fraction of ~12%. However, while for implanted fluences up to 4E12 cm-2 hardly any change at all was observed in the interstitial fraction in undoped and in n-GaN, in p-type GaN following implantation of 1E12 cm-2 of 27Mg it decreased to the ~12% level found for undoped GaN; in as-grown Mgdoped GaN, a similar decrease occurred but already at a fluence of 2.5E11 cm-2, i.e. around four times faster. Raising the implantation temperature above RT, the amount of interstitial 27Mg initially increased in all types of samples, most pronounced in both Mg pre-doped samples, where interstitial fractions around 30% were reached for ultra-low fluence implantation at 400°C.

Finally, implanting at temperatures above 400°C progressively converted interstitial 27Mg to substitutional Ga sites in all doping types; detailed Arrhenius curves were measured, from which for all four sample types the activation energy for migration of interstitial Mg was estimated between 1.3 and 2.1 eV.

These results are being interpreted within the framework of Fermi-level dependence of the formation of interstitial vs substitutional Mg. The amount of interstitial Mg formed is highest when the Fermi level is low in the band gap, i.e. in p-type material. However, with increasing fluence the implantation-related defects push the Fermi level towards the middle of the band gap, which reduces the amount of interstitial Mg to levels which are identical to undoped material. The fact that this also happens in Mg-predoped samples that were not previously activated indicates that these were actually also p-type, however, with smaller hole concentration since the effect was faster. The observation that the amount of interstitial Mg initially increases with temperature can be explained by the fact that implantation at elevated temperatures creates less defects so that damage-related shifts of the Fermi level are less pronounced. We also have indications that the amount of interstitial Mg is influenced by changes in the Fermi level due to positive charges building up on the GaN surface during implantation.

[1] U. Wahl, L.M. Amorim, V. Augustyns, A. Costa, E. David-Bosne, T.A.L. Lima, G. Lippertz, J.G. Correia, M.R. da Silva, M.J. Kappers, K. Temst, A.Vantomme, and L.M.C. Pereira: "Lattice location of Mg in GaN: A fresh look at doping limitations", Physical Review Letters 118 (2017) 095501.

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