IDENTIFICATION OF $\mathbf{Be_{Ga}}$ IN GaN WITH POSITRON ANNIHILATION

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One of the main challenges in manufacturing of wide-band semiconductors is controlling the *p*-type doping level. In the case of GaN, the most commonly employed *p*-type dopant has been Mg. However, the limitations related to the saturation and subsequent decrease of hole concentrations at [Mg] higher than 10^{20} cm^{-3} set the demand to employ an alternative acceptor [1]. Another group II element, namely Be, was studied as an alternative in the past, but is now thought to be an even deeper acceptor than Mg [2]. However, Be-doped GaN (that gives broad yellowish emission) grown on top of a blue GaN light-emitting diode has been recently proposed to be useful for the creation of an all-nitride white light emitter [3]. Detailed understanding of the behavior of Be in the GaN lattice is hence of utmost importance.

We present results obtained by positron annihilation spectroscopy in Be-doped and Be-/Mg-codoped high-nitrogen-pressure grown bulk GaN crystals [4] and Be-doped GaN thin films grown by molecular beam epitaxy [5]. Positron lifetime as well as Doppler broadening experiments in both conventional and coincidence modes were performed. In addition, the positron annihilation signals were calculated with state-of-the-art first principles methods [6] for a wide variety of defects that may act as positron traps in GaN.

Through comparison of experiments and theory, we identify the Be on Ga site (Be_{Ga}) in GaN as the dominant form of occurrence of Be in as-grown samples. This defect is able to trap positrons in spite of the small open volume associated with it, similarly as the Li_{Zn} in ZnO [7]. The positron lifetime is only a few picoseconds above the GaN lattice lifetime for Be_{Ga} (comparing to V_{Ga}, for which the defect-specific lifetime is 70 – 80 ps longer). The coincidence Doppler fingerprint of Be_{Ga} is very distinct and matches perfectly that obtained by theoretical calculations. Annealing or growth at high temperature (above 900 °C) results also in efficient incorporation of Ga vacancies into the samples. At high enough temperatures, Be interstitials may be formed making the material *n*-type and increasing the formation probability of acceptor-type Ga vacancies.

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