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Lattice location of 27Mg in GaN: latest results using the emission channeling technique

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Mg-doped p-type GaN is nowadays a core component of many optoelectronic devices which we find in our homes, e.g. LEDs for solid state white lighting or blue lasers. Yet there are some basic properties related to p-type doping of GaN that are still poorly understood and also limit the performance of devices. One such major problem is an inherent doping limit: once the Mg concentration in GaN surpasses ~1E19-1E20 cm3, further introduction of Mg does not lead to an increase in the hole concentration. Recently a theory has been put forward [1] that explains this behaviour by suggesting an amphoteric nature of Mg: once the doping limit has been reached, additional Mg atoms are not incorporated on substitutional Ga sites any more (where they act as acceptors) but on interstitial sites (where they form compensating double donors).

The emission channeling technique with short-lived isotopes (EC-SLI) is an experimental method that gives direct information on the lattice location of radioactive isotopes implanted into single crystals. Using the isotope 27Mg (t1/2=9.5 min) produced at CERN's ISOLDE facility hence offers the unique opportunity of studying the Mg lattice location in GaN and other nitride semiconductors such as AlN and InN.

In this contribution, recent results on the lattice location of 27Mg ion implanted in different doping types of GaN (undoped, Si-doped n-type, Mg-doped p-type, Mg-doped as grown) will be discussed. We give direct evidence for the amphoteric nature of Mg, which is proven by the simultaneous occupation of substitutional Ga and interstitial sites. After implantations between room temperature and 300℃, the majority of 27Mg occupies the substitutional Ga sites, however, significant fractions were found on interstitial positions ~0.6 Å from ideal octahedral sites. The interstitial fraction of Mg was correlated with the GaN doping character, being highest (up to 30%) in samples that were doped p-type with 2E19 cm3 stable Mg during epilayer growth, and lowest in Si-doped n-GaN, thus giving direct evidence for the amphoteric character of Mg. Implanting above 400℃ converts interstitial 27Mg to substitutional Ga sites, which allows estimating the activation energy for migration of interstitial Mg as between 1.4 and 2.1 eV.

[1] G. Miceli and A. Pasquarello: "Self-compensation due to point defects in Mg-doped GaN", Phys. Rev. B 93 (2016) 165207

Primary author: WAHL, Ulrich (Instituto Superior Tecnico (PT))

Co-authors: VANTOMME, André (KU Leuven, Instituut voor Kern- en Stralingsfysica); GRANADEIRO COSTA, Angelo Rafael (Instituto Superior Tecnico (PT)); DA SILVA, Daniel (Universidade do Porto (PT)); DAVID BOSNE, Eric (Instituto Superior Tecnico (PT)); MARTINS CORREIA, Joao (Instituto Superior Tecnico (PT)); TEMST, Kristiaan (KU Leuven, Instituut voor Kern- en Stralingsfysica); PINTO DE ALMEIDA AMORIM, Ligia (Katholieke Universiteit Leuven (BE)); DA COSTA PEREIRA, Lino Miguel (KU Leuven (BE)); CASTRO RIBEIRO DA SILVA, Manuel (Instituto Superior Tecnico IST); KAPPERS, Menno J. (University of Cambridge, Cambridge Centre for Gallium Nitride); DE LEMOS LIMA, Tiago Abel (KU Leuven (BE)); AUGUSTYNS, Valerie (K)

Presenter: WAHL, Ulrich (Instituto Superior Tecnico (PT))

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