Density Functional Theory study on the incorporation of In, Mg and Si atoms on GaN(0001) surface in MOVPE growth conditions

Pawel Kempisty[1], Pawel Strak[1] and Stanislaw Krukowski[1]

[1] *Institute of High Pressure Physics, Polish Academy of Sciences, Sokolowska 29/37, 01-142 Warsaw, Poland*

Using density functional theory (DFT) calculations we analyzed processes occuring on GaN(0001) surface under mixed coverage composed of NH_2 radicals and NH_3 admolecules typical for the growth of GaN layers and crystals by MOVPE and HVPE methods. Recently we observed that the adsorption and desorption energy is strongly dependent on the availability of empty quantum states and pinning of the Fermi level at the surface [1]. If the quantum states at the semiconductor surface strongly pin the Fermi level, the doping type of the semiconductor bulk has no impact on the process: the adsorption/desorption energy is approximately the same for the n-type and p-type, similarly to metal surfaces. A different behavior is observed when the surface complies with the electron counting rule (ECR) so that Fermi level is not pinned and therefore determined by the dominating point defect states in the bulk. Under such conditions, the adsorption energy is dependent on the doping of material (p-type or n-type). In this work we present this phenomenon with regards to adsorption of indium and primary dopants, i.e. magnesium and silicon at the GaN(0001) surface covered with 25% of NH_3 molecules and 75% of NH_2 radicals. A single magnesium atom is very weakly adsorbed on the surface of n-type material while the Mg-H pair is very strongly bound to the surface. This result is fully consistent with experimental observations of the existence of Mg-H complexes after growing Mg-doped GaN. Hydrogen attachment to In adatoms increases desorption of indium from surface, which may be one of the factors leading to much severe InGaN growth conditions than for GaN.

[1] S. Krukowski, P. Kempisty and P. Strak *J. Appl. Phys.* **114**, 063507 (2013).