Limitation to p doping in GaN due to self-compensation

Alfredo Pasquarello*

Chaire de Simulation à l'Echelle Atomique (CSEA), Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

We address point defects susceptible to cause charge compensation upon Mg doping of GaN using hybrid density functional theory. We determine the free-energy of formation of the nitrogen vacancy and of several Mg-related defects. The entropic contribution as a function of temperature is determined within the quasiharmonic approximation. We find that the Mg interstitial shows a noticeably lower free-energy of formation than the Mg substitutional to Ga in p-type conditions. Therefore, the Mg impurity is amphoteric behaving like an acceptor when substitutional to Ga and like a double donor when accommodated in an interstitial position [1,2]. In particular, we find that the diffusion of the interstitial Mg^{2+} ion is hampered by high energy barriers of the order of 2 eV [3]. The hybrid-functional results are then linked to experimental observations by solving the charge neutrality equations for semiconductor dominated by impurities. We show that a thermodynamic equilibrium model is unable to account for the experimental hole concentration as a function of Mg doping density, due to nitrogen vacancies and Mg interstitials acting as compensating donors [2]. To explain the experimental result, which includes a drop-off of the hole concentration at high Mg densities, we thus resort to non-equilibrium models. We show that either nitrogen vacancies or Mg interstitials could be at the origin of the self-compensation mechanism. However, only the model based on interstitial Mg donors provides a natural mechanism to account for the sudden appearance of self-compensation. Indeed, the amphoteric nature of the Mg impurity leads to Fermi-level pinning and accounts for the observed drop-off of the hole concentration of GaN samples at high Mg doping. Our work suggests that current limitations in p-type doping of GaN could be overcome by extrinsically controlling the Fermi energy during growth.

*Work performed in collaboration with Giacomo Miceli.

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[2] G. Miceli and A. Pasquarello, *Phys. Rev. B* **93**, 165207 (2016).
[3] G. Miceli and A. Pasquarello, *Phys. Status Solidi RRL* **11**, 1700081 (2017).