Numerical drift-diffusion modeling of nitride laser diodes: dopant-related optical losses, multi-stable carrier transport, and a glance at crystal vision

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Macroscopic simulation of carrier transport in group-III nitride optoelectronic devices provides vital insight into efficiency-limiting mechanisms, but it poses severe challenges across both numerical and physical domains. This seminar presents recent collaborative research carried out at the Institute of High Pressure Physics PAS, focusing on two central topics: the numerical modeling of dopant-related optical absorption in nitride laser diodes (LDs) and a robust numerical formulation for resolving multi-stable, S-shaped transport regimes in polar heterostructures. In addition, a brief glance will be given to initial materials informatics and computer vision workflows developed for ammonothermal GaN crystal growth.

The main part of the talk addresses parasitic optical losses in high-power (In,Al)GaN laser diodes, which critically restrict slope efficiency and light extraction. Conventional simulation approaches typically treat optical losses using static, spatially uniform absorption coefficients, neglecting the spatial coupling between carrier transport and local defect states. Here, we present a unified model that couples 1D drift-diffusion transport equations with quasi-Fermi-level-dependent dopant ionization profiles. We demonstrate how forward-bias quasi-Fermi levels directly govern the localized ionization of Si donors in the n-type region and Mg acceptors in the p-type region. Crucially, the model reveals that unintentional donor compensation in the p-type layers severely accelerates parasitic optical absorption by driving higher Mg ionization, despite the low thermal activation baseline of magnesium ($\sim$1%). This provides a rigorous theoretical explanation for why undoped waveguide designs suppress internal absorption by up to an order of magnitude and highlights the decisive role of crystal growth quality and defect reduction in maximizing optical performance.

The second focus explores the numerical treatment of abrupt polarization charges at heterointerfaces and the emergence of multi-stable operating states. In polar heterostructures, localized carrier accumulation and dynamic screening at polarization barriers can induce thyristor-like switching and S-shaped current-voltage (I-V) characteristics with negative differential resistance (NDR). Because bias voltage is multi-valued across the fold, conventional voltage-controlled (Dirichlet) sweeps cannot resolve the intermediate branch: stepping the voltage past a turning point leads either to solver divergence—since the previous branch state is too far from any valid solution—or to abrupt hysteretic jumps that bypass the fold entirely. To overcome this limitation, we formulate a current-controlled scheme that replaces contact Dirichlet conditions with physically consistent Neumann boundary conditions for the electrostatic potential and quasi-Fermi levels within a composite discontinuous Galerkin method. By parameterizing the solution path directly by the monotonically varying total current density, the scheme maintains stable convergence across the entire S-curve, reconciling numerical predictions with experimentally observed delayed turn-on voltages and electrical hysteresis.

Finally, bridging device simulation with substrate technology, we offer a brief glance at ongoing work within the MAB "GaN-Unipress" Materials Informatics initiative (WP4). We highlight early Python and OpenCV prototypes developed for automated crystal contour extraction, area measurement, and polarized-light defect screening in the Ammono pilot line, outlining how these tools feed into a "Digital Crystal" framework linking growth history with material quality.