Project 6.1 Ab initio modeling of point defects in III-nitride semiconductors

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Background:

The project will be theoretical research focused on the thermodynamics of point defects in gallium nitride. It is commonly known that in the real experiment the concentrations of point defects are strongly dependent on the direction of growth, i.e. the crystallographic orientation of the surface on which the growth takes place. However, in the world literature equilibrium models based on bulk properties are dominant. The pioneering aspects of the project will involve determining the behavior of the selected point defects in the nanometric areas close to the surface. The phenomena occurring at the atomic level will be investigated. The research will be carried out on the basis of quantum-mechanical calculations from first principles as well as statistical physics and thermodynamics. Most of the calculations will be made based on the density functional theory DFT. The results will include the energy levels of defects, the energies of their formation and diffusion barriers. Additionally, the change of free energies as a function of temperature will be determined on the basis of phonon spectra, also calculated by the DFT method. The behavior of such technologically important dopants as Ge, Mg and C will be analyzed. Controlling these dopants is crucial for achieving high-quality n-type, p-type or semi-insulating material. The project will also include research on GaN doped with atoms of group V elements: As and P, and their co-doping with Mg. It is planned to compare the formation energy and electronic properties the same point defects at various surfaces under growth conditions by different epitaxial methods.

Aim:

The project focuses on improving GaN growth and doping models. Point defects in crystals are governed by the fundamental thermodynamic principles and present project will help to better understand them. The research will provide basic thermodynamic parameters and information which is not straightforwardly accessible in growth experiments, e.g. the relationship between the microscopic atomic state of a surface and the possibility of incorporating foreign atoms or the rules of selecting a lattice site.

Requirements:

- completed studies in the field of physics, materials engineering, chemistry, computational materials sciences, or related,
- knowledge of solid state physics, semiconductor physics, quantum mechanics, thermodynamics and statistical physics,
- ability to work in Linux system and programming in Python/C/Fortran,
- knowledge of English to a degree that enables the understanding professional literature, presenting research results and writing scientific publications.