Gallium nitride (GaN) is considered one of the most promising candidates for high-power electronic devices. Power semiconductor devices are critical for future energy infrastructure around the world. GaN-based power devices are currently the alternative with the potential to meet future demands. Their full triumph depends on successful solutions to the materials problems that are partially analyzed and solved in this project.

Silicon (Si) is the main dopant for obtaining highly conductive gallium nitride (GaN) in epitaxial technologies. Silicon is also implanted into GaN to obtain selected areas of higher free carrier concentration in electronic devices. However, the diffusion coefficient of Si in GaN, as well as its activation energy and solubility limit have not been determined yet. At epitaxial temperature, of the order of 1000-1100°C, strong diffusion effects never occur in GaN. As a rule, diffusion begins at 2/3 of the melting temperature of the compound in question. It was shown that the melting point of GaN exceeds 2300°C. Hence, diffusion processes begin at 1300-1400°C. At such high temperature, GaN decomposes under atmospheric pressure. If the process of diffusion of a given impurity in GaN is considered, high temperature and therefore also high nitrogen pressure, which prevents the GaN surface decomposition, are needed. Only thanks to ultra-high-pressure annealing (UHPA) technology it is possible to study the diffusion of various elements in GaN.

The main goal of this work is to analyze the diffusion process of Si in GaN of the highest structural quality and purity. Gallium nitride crystals grown by halide vapor phase epitaxy on ammonothermal GaN substrates will be used. The diffusion phenomenon in four basic crystallographic directions for GaN will be examined. UHPA technology will be used to force the Si diffusion in HVPE-GaN. UHPA provides stability of GaN at high temperature up to 1650°C by applying hydrostatic nitrogen pressure up to 2 GPa.

Silicon diffusion in GaN will be studied by annealing Si_xN_y-coated and Si-implanted GaN (both treated as infinite sources of the species) at high temperature using the UHPA technology. By analyzing the depth profiles of Si in GaN (obtained by Secondary Ion Mass Spectrometry; SIMS) the diffusion coefficients, activation energies and solubility limits will be determined. Fitting of SIMS profiles will be performed with the Finite Difference Method. The depth profile alone is not sufficient to identify the mechanisms of diffusion. A detailed analysis has to include a direct comparison of the experimental profiles with numerical solutions of the full partial-differential-equation system.

The use of two Si sources for GaN will allow for a better understanding of the role of point defects, particularly gallium and nitrogen vacancies, in the diffusion process. It is well known that ion implantation generates Frenkel and Schottky defects in the crystal structure. They are, in turn, not generated during diffusion of any element from a sputtered layer. During the proposed project such experiments will be carried out for the first time for GaN and Si. Attention should also be paid to using GaN of high structural quality and purity. Both threading dislocations (TDs) and impurities will not strongly interfere with the diffusion process. The influence of TDs and impurities will, therefore, not be taken into account, which should facilitate the analysis of the diffusion process itself.

For the first time, the activation energies, diffusion coefficients and solubility limits of Si in GaN of the highest structural quality and purity will be determined. The effect of point defects on the diffusion process will also be taken into account. The proposed research will be purely scientific and absolutely novel. This will also allow a better design of electronic structures based on Si-doped nitrides.