Summary

Wpływ defektów punktowych na termiczną stabilność układu wielu studni kwantowych InGaN/GaN

This dissertation presents the results of modeling and analysis of the possible processes occurring at different stages of the fabrication of InxGa1−xN/GaN thin films grown by metal organic vapor phase epitaxy (MOVPE). This work is theoretical in nature and is based on quantum mechanical calculations using density functional theory (DFT) with supercell and supergrid models in the generalized gradient approximation (GGA). For the purpose of the dissertation, a new methodology was developed to calculate the height of energy barriers for the diffusion of point defects through the interface of two materials. First, simulations of the diffusion of VN, VGa and VIn vacancies in InxGa1−xN systems were performed as a starting point for the analysis of the thermodynamic processes occurring in these systems. An energetic "hierarchy"of barriers to individual point defect migration was observed. Furthermore, much lower Energy barriers were observed for InGa+VGa complex migration than for a single VGa vacancy. In the next step, using the harmonic approximation and the harmonic transition state theory, the heights of the migration energy barriers for In and Ga atoms diffusing in InxGa1−xN systems (x = 0; 0.11; 0. 22), the vibrational frequencies of InxGa1−xN systems in the presence of migrating point defects, the temperature dependence of the defect migration energy barriers, and the diffusion coefficients of Ga and In atoms migrating in InxGa1−xN systems have been calculated. Based on the analysis of the diffusion of point defects both in the bulk InxGa1−xN system and on the InxGa1−xN/GaN interfaces as well as the temperature-dependent diffusion coefficients, a model of the thermal decomposition of the InGaN/GaN multiquantum well system using the Kirkendall effect was proposed.