Abstract

Title of dissertation:

Modelling of light emitting diodes and laser diodes based on nitride heterostructures

Existing computational schemes employed for modelling of optoelectronic devices are mostly based on semi-classical drift-diffusion equations that are solved for the whole device. On the other hand, the active regions of such devices are modelled using quantum mechanical description to obtain the rates of optical transitions. The aim of the present thesis was (i) to assess main physical mechanisms that influence current-voltage characteristics of optoelectronic devices based on nitride heterostructures, and (ii) to propose the modifications of the computational scheme that could allow for reliable modelling of electric characteristics of such devices. Owing to the strong electric fields existing in the nitride heterostructures (originating from the strong piezo- and pyro-electric character of these materials), large band gaps (in comparison to the analogous devices for 'red' optoelectonics based on arsenides), and large number of narrow quantum wells and barriers, the nitride devices constitute extremely difficult object for the solution of the drift-diffusion equations. In the most cases, the standard algorithms of solution of these drift-diffusion equations do not lead to convergent solutions for devices containing nitride heterostructures. Therefore, the first task undertaken in this thesis was to develop a method of solution of drift-diffusion equations that could provide convergent solutions for systems based on nitride heterostructures. The very efficient method of integration of drift-diffusion equations was developed and implemented in the numerical package next**nano**^{3}, which constituted the basic research tool of the thesis.

The second important task was to investigate various recombination mechanisms. The recombination model taking into account the presence of the strong electric fields was implemented in the next**nano**^{3} code. Employing the next**nano**^{3} code with the modifications mentioned above, modelling of realistic structures applied in the light emitting diodes (LEDs) and laser diodes (LDs) fabricated in the Institute of High Pressure Physics of the Polish Academy of Sciences, was performed.

The third important issue considered in the thesis was the calculation of the current in the part of device containing multiple quantum wells employing quantum mechanical approach. The currents calculated on the basis of quantum mechanical schemes were compared to the predictions of the semi-classical drift-di_usion approach. For the quantum mechanical calculations of the current, the scheme for calculation of the transmission coefficients was developed and then employed for the calculation of current-voltage characteristics of the considered nitride structures. The performed studies clearly demonstrate that the reliable modelling of the optoelectronic devices based on nitride heterostructures cannot be performed employing solely drift-diffusion equations. The present thesis provides solid basis for development of an hybrid model of devices, where active regions are described using quantum mechanical approach, and other 'classic' parts (which are mostly used to transport carriers to the active region) are treated through drift-diffusion equations.