Theory and modeling of semiconductor structures with modulated magnetization

This thesis provides the computational scheme that allows for reliable modeling of wide class of semiconducting structures, also with modulated magnetization, on the quantum-mechanical and/or semi-classical Thomas-Fermi approach levels employing continuous methods. The scheme is based on the existing simulation tool nextnano^3, however the three new crucial features have been implemented into the code: (i) the Burt-Foreman version of the ***k.p*** method with unique ordering of operators that avoids the artifacts of the so-called symmetrized Hamiltonians, (ii) introduction of the p-d couplings to the ***k.p*** Hamiltonian that describes the interaction between carriers and the localized moments and accounts for the appearance of spontaneous magnetization, and (iii) treatment of superlattices. The developed code has been carefully tested and employed further for the studies of magnetic GaAs/AlGaAs/(Ga,Mn)As heterostructructures and InAs/GaSb superlattices. These studies provide physical insight and increase the understanding of these two important classes of systems. In particular, this thesis provides quantitative predictions of the electrical field influence on the Curie temperature of the gated GaAs/AlGaAs/(Ga,Mn)As heterostructures. The main physical mechanism is the tuning of the hole density with the external bias. The bias induced increase of the hole density leads to the increase of Curie temperature in the layer of dilute magnetic semiconductor (Ga,Mn)As. These studies reveal that the roughness of the gate/oxide interface introduces the strong scattering of carriers and the semi-classical approach is more suitable for treatment of these systems and also leads to better agreement with experimental data. The studies of InAs/GaSb based systems clearly demonstrate that the diffusion of In and Sb atoms into neighboring regions observed experimentally has strong influence on the electronic structure and absorption profiles of these systems.