Belarusian State University

Faculty of Applied Mathematics and Computer Science

Modeling of the Effect of External Electric and Magnetic fields on Electronic States near Semiconductor Interface

Master Thesis

Levchuk E.A.

Advisor: Makarenko L.F.

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Resume

In this work, numerical simulations of the effect of external electric and magnetic fields on the states of shallow donor located near the surface of semiconductor are carried out. During the simulations problem for the Laplace equation and eigenvalue problem for the stationary Schrödinger equation are solved.

Theoretical analysis of convergence rate of finite element method for considered problems is performed. A way of implementation of the method for problems with discontinuous boundary conditions is also proposed. Approximation order of finite element method is studied and the effect of errors of electric field calculations on solving problem for the Schrödinger equation is investigated.

Modeling of energies and wave functions of ground and lower excited states are conducted using finite element method. Emphasis in the modeling is placed on parameters of control of electron shuttling from the donor to the gate: critical gate potential, at which the shuttling takes place, and minimum gap between ground and first excited state energies.

The dependences of electron ground state energies in field of disc-shaped gate on gate potential are determined for different boundary conditions for electrostatic potential. The obtained dependences can be used to estimate the critical potential when the donor is infinitely distant from the gate, and corresponding formulae are proposed. It has been shown that these estimates are applicable for finite distances between the donor and the gate if potential difference on the donor and the gate is used as control parameter instead of gate potential.

The dependences of ground and lower excited states on gate potential in donor-gate system are studied. It has been found that anticrossing behavior of energy levels takes place for adjacent levels. Minimum point of the gap between ground and first excited state energies can be used to calculate the critical potential. This method has been used to obtain the dependences of the critical potential on gate diameter and donor position.

Empirical formulae for the critical potential as a function of gate diameter are proposed for infinite distance between the donor and the gate. The effect of uniform external electric field on electronic spectrum is also considered. Several qualitative differences between the cases of uniform and nonuniform external fields are revealed.

It has been found that donor position does not affect the critical potential difference on the donor and the gate, while the minimum gap demonstrates exponential dependence on donor position. The dependence of the minimum gap on gate diameter is also defined.

Trial function of a simple form for variational method is proposed in the case when the gate is surrounded with dielectric. The quality of the trial function has been determined by comparing with the results obtained by finite element method. This trial function gives a simple method to calculate the critical potential.

The effect of electron effective mass, magnetic field, dielectric thickness, and image charges on the characteristics of the system is also studied.

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