Belarusian State University

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Calculation of Electronic Spectrum of Semiconductor Nanostructures with Finite Element Method

Diploma Work

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Resume

The work presents the results of the study of applying finite element method to the quantum mechanical modeling of electronic states near semiconductor interface. During the modeling boundary value problem for the Laplace equation and eigenvalue problem for the Schrodinger equation are solved.

The problem for the Laplace equation is considered in multilayered medium, the existence and uniqueness of solution for the problem are proved. Several analytical expressions for electrostatic potential are obtained for different boundary conditions and geometrical parameters of the medium. To solve this problem, an algorithm for finite element method is also proposed and implemented in Matlab. Theoretical analysis of the convergence rate of finite element method for electrostatic problem in multilayered medium is performed, including the problem with discontinuous boundary conditions.

Finite element method is also used to solve eigenvalue problem for the stationary Schrödinger equation. FEM is implemented in Matlab with rebuilding the grid to minimize error in solution of the Schrödinger equation. The approximation order of FEM is studied. It has been found that error of the solution of the problem for the Schrödinger equation is affected not only by FEM error, but also by error of the electric field calculations. It has been shown that the corresponding error has the first order.

To solve the problem for the Schrödinger equation, variational method with different trial functions is also used. The results of application of variational method are compared with the corresponding results obtained using FEM. On the basis of this comparison, trial function with parameters depending on gate potential is proposed, which makes it possible to simplify the calculations.

The results of simulations of electron states in the field of the disc-shaped gate and in the donor-gate system are also presented. In particular, the dependence of the ground state electron energy on gate potential in the absence of donor potential influence is defined. It has been shown, that this dependence can be used to estimate critical potential for infinite distance between the donor and the gate.

Several methods for calculation of the critical potential for finite distances between the donor and the gate are proposed. The dependence of critical potential on system geometry is obtained. The effect of image charges on electronic states is also studied.

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