Convergence Studies in a Coupled Self-consistent Poisson-Schrödinger Equation for Complex Quantum Well Nanostructures

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BIOGRAPHY
Roberto Yuji Tanaka holds a Master’s degree in Applied Computing from the Brazil’s National Institute for Space Research (2008). Nowadays, he is working in his doctoral thesis in the Space Science and Technology program of the Aeronautic Technical Institute (ITA). He works since 2002 at Brazilian Air Force's Department of Aerospace Science and Technology and has experience in computational science, with emphasis on numerical methods and optimization applied to nanostructured semiconductors such as quantum well and quantum dots.

TECHNICAL ABSTRACT
In this work we present a robust self-consistent computer procedure to solve the coupled Schrödinger and Poisson equations, based on the Finite Element Method, to help the design and the analysis of quantum well based devices.

Keywords: Numerical methods, finite element methods, nanotechnology, nanostructured semiconductors, doping.

INTRODUCTION
In order to consider the presence of ionized impurities in quantum well (QW) structures, one approach, usually adopted in literature, is a self-consistent computation, solving a pair of coupled partial differential equations (PDEs): the Poisson and the Schrödinger equations. Iterative self-consistent solution of the coupled Poisson-Schrödinger equations is a nonlinear problem and may require a more elaborated procedure in order to achieve the solutions convergence [1]-[2]. In these systems even the smallest change in the electric potential energy can cause difficulties in the evaluation of the Fermi level because either the energy oscillates among iterations or the process can converge to wrong results. These small changes lie in the limited computer precision, which can provoke round errors, unbalancing the charge distribution in a symmetric structure and resulting in charge bouncing from one iteration to the other.

In this work, a procedure presenting robust and stable convergence behavior is presented. It is an improvement of the self-consistent procedure presented in [3]. The pair of coupled PDEs is solved by the one-dimensional Finite Element Method, 1D-FEM, using a weak coupling schema. Some results of the simulation of multi quantum wells (MQW) with high values of doping concentration are presented.

POISSON-SCHRÖDINGER SELF-CONSISTENT ALGORITHM
The self-consistent procedure is briefly discussed in the next lines. Initially, the Schrödinger equation, with the conduction band potential energy profile is solved and the wave functions are obtained. The wave functions are used to calculate the Fermi energy and, assuming that the structure presents neutrality of charges, the charge distribution (electrons and ionized doping atoms) is calculated, which in turn is inserted into the Poisson equation to give the charge generated potential. The Schrödinger equation is solved again to the new potential obtained from the original one plus the result obtained from the Poisson equation, closing the cycle. This iterative process continues till a given convergence criteria is satisfied. In order to achieve a more stable iterative process the charges distribution and the potential are accumulated in the 1D-FEM internal matrices. This process dampen, over the iterations, the possible huge variation of the total potential and charges mobility, respectively. In this way, the changes in the computed Fermi energy is dramatically reduced conducting to a smoother convergence curve. The accumulated matrices are, during the iterations, gradually taken to the correct value. This procedure is equivalent to the inclusion of a diffusive term in the Poisson equation which is eliminated naturally during the iterative process. The algorithm works in all nanostructures studied by this group [3] [4], however, in a complex symmetric doped MQW structure, this procedure was unable to avoid the small

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concentration of charges in one side of the structure. As an undesired result of the inclusion of the diffusive term, it can take a huge number of iterations to these small charges be distributed equally on the two halves of the structure as expected. Depending on the convergence threshold adopted, this can make the process halt in a wrong result.

To overcome this troubled cases, it was observed that in this kind of complex symmetric structure, introducing the actual Poisson charges instead of the accumulated charges in the iterative process in stepped intervals gives a better stabilization to the convergence. This process is here named as X. To illustrate the effect of the introduction of Process X in the self-consistent algorithm, the convergence curve of a Al0.3Ga0.7As/GaAs symmetric MQW structure with ten wells 10 nm wide and contact layers is showed in Figs. 1 and 2. The wells are separated by 30 nm barriers. All barriers are doped with Si (density of 3.0x10^{15} cm^{-3}). Fig. 1 shows the convergence curve obtained in the self-consistent computation of the symmetric MQW without the Process X. Note that the convergence curve displays bumps that are associated with the small quantity of charges going from one side of the structure to another. With the use of Process X, Fig. 2, there are some oscillations in the beginning of the iterative calculation but the bumps lessen until disappear completely. Fig. 3 presents the charge distribution achieved (a) without and (b) with the Process X, assuming total ionization. Note that without Process X the solution converges to a wrong charge distribution. Tests with the computation of depletion regions were also accomplished in order to understand the impact of the tentative solutions to enhance the convergence process.

The combined techniques applied have allowed stable convergence of self-consistent computations, even for complex QW structures. Consistent charge distributions, energy of subbands and wavefunctions are obtained. However, a general numerical algorithm that is independent of the complexity of the nanostruclture is necessary in order to apply this code for the computational optimization of nanostructures, which is already in progress [4].

REFERENCES


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