Software Tools for the Design and Analysis of Quantum Well, Quantum Wire and Quantum Dot Devices

Roberto Y. Tanaka[1], **Stephan Stephany**[2], **Angelo Passaro**[1], **Nancy M. Abe**[1], **José M. Villas-Bôas**[1], **Gustavo S. Vieira**[1]

[1]Divisão de Física Aplicada – Instituto de Estudos Avançados (IEAv/CTA) Caixa Postal 6.044 – 12.228-970 – São José dos Campos – SP – Brazil

[2]Laboratório Associado de Computação e Matemática Aplicada – Instituto Nacional de Pesquisas Espaciais (INPE) – São José dos Campos – SP – Brazil

roberto@ieav.cta.br

Abstract. *In this work we present a set of computer codes based on the Finite Element Method intended to help the design and the analysis of infrared photodetectors based on semiconductor quantum wells and quantum dots. Our codes are capable of handling both arbitrary potential and effective mass profiles and they take into account the strain induced by lattice mismatch between different materials. In the present version, the computer codes allow the computation of eigenvalues, eigenvectors and oscillator strain for optical transitions.*

1. Introduction

The first infrared photodetector based on intersubband transitions in semiconductor quantum wells was demonstrated in 1987 [Levine et al. 1987]. Since then, a lot of research has been put forward to develop this technology further, and today large format and high uniformity GaAs focal plane arrays based on such technology are already available on the market [Goldberg et al. 2005]. The success of such technology is mainly due to its relative low cost, high pixel uniformity, selectivity and design flexibility.

Infrared photodetectors based on intraband transitions in quantum dots (QDIPs) should, in principle, out-perform the ones using quantum wells (QWIPs), because of the possibility of absorbing normal incident light and operating at higher temperatures due to the electron longer lifetimes. Although the performance of QDIPs has improved considerably in the last few years, there is still much to be done before the QDIPs seriously compete with the QWIPs.

The properties of both kinds of detectors are dependent on a fine adjust of both the material composition and thickness of each layer that compound the detector structure. In this work, we present the development of computer codes that allow the evaluation of the electronic states in quantum dots and wells and respective oscillator strain for photon absorption. The codes are intended to help in the design of QWIPs and QDIPs.

2. The Computer Code

The computer code developed in this work is part of an effort to develop a multiphysics computer program, named LEVSOFT [Abe et al. 2006]. The module developed for the analysis of multi-quantum wells (MQW) is named QWS. QWS allows the definition of

the parameters of a MQW, such as, the thickness and the sequence of the material layers that compound the device, and it computes both the effective mass and the potential of confinement of the conduction band of each layer. It also computes a set of eigenenergies and eigenstates associated to the MQW and the oscillator strain, the probability of absorbing incident radiation between two energy levels of the MQW.

A simple user friendly graphic interface was developed in order to allow the definition of the layer thicknesses and the materials composition (binary, ternary and quaternary alloys of III-V compound semiconductors). The material parameters of the alloys were obtained from [Vurgaftman et al. 2001]. This version of the program also allows the use of different parameters inserted manually. The graphic user interface allows the definition of periodic structures easily. The conduction band profile, including the strain due to the lattice mismatch between different materials, is automatically computed when it is needed.

The potential of confinement of each layer, the eigenvalues and eigenvectors, are also presented graphically in order to allow their analysis. The eigenfunction outputs are presented superposed to the energy level of the respective quantum state. The visualization options allow putting in evidence each one of the eigenvalues and eigenfunctions.

We implemented other two modules that allow the design and analysis of quantum wires and quantum dots. The quantum dot modules implemented use a 2D-axial FEM.

3. Mathematical Formulations: Finite element model - FEM

Consider the Schrödinger's equation in the effective mass approximation for a conduction band electron in layered quantum heterostructure . The envelope functions satisfy the equation:

$$-\frac{\hbar^2}{2}\left(\nabla\frac{1}{m^*(\vec{r})}\nabla\right)\Psi(\vec{r})+V(\vec{r})\Psi(\vec{r})=E\Psi(\vec{r}), \tag{1}$$

Here, $\Psi(\vec{r})$ represents the wave function in the structure, $m^*(\vec{r})$ is the effective mass and $V(\vec{r})$ is the effective potential energy seen by one electron in the conduction band. For the moment, each layer is assumed to have a uniform composition and so, a constant $V(\vec{r})$ and effective mass. It is important to point out that $V(\vec{r})$ is the superposition of the potential energy due to the conduction band offsets at interfaces between layers and the potential energy that arises from the presence of ionized donors and the released free charges. In this work, we consider only the potential energy due to the conduction band offsets at interfaces between layers.

In the FEM, the wave functions are expanded inside each element in terms of a compact set of base functions, N_j,

$$\psi=\sum_{j=1}^{n_p}N_j\psi_j, \tag{2}$$

with n_p the number of nodal points in the finite element and ψ_i are the value of the wave function computed in each nodal point. The base functions have the following properties on the nodal points: $N_i^{(\gamma)}(\vec{r}_j)=\delta_{ij}$, where δ_{ij} is the Kronecker's delta. The base functions for a determined element γ are valid only in the limits of this element. The

value of ψ inside an element is obtained from Eq 2. In this work we use finite elements of first order (linear base functions, with continuity C^0) or of second order (quadratic base functions, with continuity C^1).

By applying the FEM, one obtain an eigenvalue system equation given by

$$-\frac{\hbar^2}{2m^*}A_{ij} + (V - E)B_{ij} = 0, \tag{3}$$

where $A_{ij} = \psi_i^* \left(\int \int_\Omega \nabla N_i^* \cdot \nabla N_j d\Omega \right) \psi_j$, $B_{ij} = \psi_i^* \left(\int \int_\Omega N_i^* N_j d\Omega \right) \psi_j$, i, j = 1,...,$n_t$ and n_t is the total number of nodal points in the domain.

The oscillator strain for the transition between two eigenstates, m and p, is computed as

$$f_{mp} = \sum_{k=1}^{n_e} \left(\int \int_{\Omega_k} \psi_{km}^* N_{km}^* r N_{kp} \psi_{kp} d\Omega \right), \tag{4}$$

where n_e is the number of finite elements.

4. Conclusions and Final Remarks

In the current stage, we have developed a computer program that allows the computation of eigenvalues and eigenfunctions for layered quantum well heterostructures. The code allows the definition of the layered structure considering band parameters for III-V compound semiconductors and some of their alloys, computes the oscillator strain, and provides a simple graphic user interface, which allows the visualization of the eigenstates.

Several test cases were executed in order to validate the FEM 1D (quantum well), FEM 2D (quantum wire) and FEM 2D-Axial (quantum dot) Schrödinger' resolution modules. The test cases were selected from the Literature and all results obtained with the implemented codes are in good agreement with it.

Together with the modules that allow the design and analysis of quantum wires and quantum dots they are a first step in the development of an integrated tool for the analysis and design of QWIP and QDIP that will allow self-consistent analysis in quantum wells, quantum wires e quantum dots structures. The implementation of a self-consistent approach for QWIP is under development.

References

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