Development of Finite Element Software Tools for QWIP and QDIP Design

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Abstract

In this work, we present a computer code based on the Finite Element Method for the design and analysis of infrared detectors based on Quantum Well and Quantum Dot technologies. This code is already prepared to handle both arbitrary potential and arbitrary effective mass profiles. In the present version, the computer codes allows the computation of eigenvalues and eigenvectors and present the results in a graphic interface. We present some results obtained with the FEM code compared to the ones obtained by the expansion of the Hamiltonian in the basis of an infinite well much larger than the region under consideration. This method is also included in the code. The code is a first step in the development of a tool that will allow self-consistent analysis in quantum wells, quantum wires e quantum dots immersed in quantum well structures.

Introduction

The Finite Element Method (FEM) has been extensively used in engineering and physics because it allows the solution of problems that present very complex geometries and inhomogeneous materials. This work is the first step in the development of a software tool, based on the FEM and auxiliary methods, for the analysis and design of QWIP and QDIP devices.

Mathematical Formulations

The Finite Element Method (FEM)

Consider the Schrödinger's equation in the effective mass approximation. The envelope function satisfy the equation:

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

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

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

$$A_{ij}=\psi_i^*\left(\iint_\Omega \nabla N_i^*\cdot\nabla N_j\,d\Omega\right)\psi_j$$

$$B_{ij}=\psi_i^*\left(\iint_\Omega N_i^*\cdot N_j\,d\Omega\right)\psi_j$$

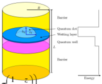
and inside each element the wave functions is expanded in terms of a compact set of base functions:

$$\psi(r)=\sum_{i=1}^{np}N_i(r)\,\psi_i$$

with np the number of nodal points in the finite element and ψ_i is the value of the wave function in each nodal point . 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).

A compreensive explanation of the FEM applied to the Poisson equation is presented in (Paes et al.,2003).

The Hamiltonian Expansion Formulation (HEF)



The solution of the Schrödinger equation in the effective mass approximation can be written as an expansion in terms of the solution of a large cylinder of length L and radii R limited by an infinity barrier:

$$\psi(r,\phi,z)=\sum_{m,n,l}C_{m,n,l}\frac{\sqrt{2}}{R\left|J_{m+1}(k_{m,n})\right|}J_m\left(k_{m,n}\frac{r}{R}\right)\frac{e^{im\phi}}{\sqrt{2\pi}}\sqrt{\frac{2}{L}}\sin\left(n\pi\left(\frac{1}{2}-\frac{z}{L}\right)\right)$$

where, $k_{m,n}$ is the n-zero of the Bessel function of order m ($J_m(k_{m,n})=0$).

The strain induced in the quantum dot due to the lattice mismatch is also taking into account.

The QWS computer program

- Windows graphic user interface;
- Layered structures: band parameters for III-V compound semiconductors and some of their alloys (Vurgaftman et al., 2001), Fig. 1;
- Handle both arbitrary potential and arbitrary effective mass profiles (FEM approach);
- Solver FEM (1st and 2nd order polynomial approximation)
- Solver HEF;
- Graphical visualisation of the potential profile, eigenvalues and eigenfunctions, Fig. 2.

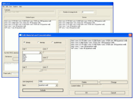


Fig.1 The interface for the definition of the quantum heterostructures.

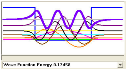


Fig.2 Graphical output showing the quantum potential, the eigenvalues (horizontal lines), and the eigenfunctions. The eigenfunctions are drawn superposed to the energy level of the respective quantum state. The visualization options allow putting in evidence each one of the eigenvalues and eigenfunctions.

QWS Code Application

Case 1: Simple rectangular quantum well - validation

The quantum well FEM code was validated comparing our results for a single quantum well with the ones obtained in a previous work in which a meshless method was employed (Machado et al., 2000). The quantum well parameters and the eigenvalues are presented in Table 1. Fig. 2 shows the eigenfunctions obtained for the quantum well of 30 nm.

Table 1- Eigenvalues for a simple GaAs/AlxGa1-xAs rectangular quantum well, effective mass $m^* = (0.067 + 0.083x)\, m_0$, where x = 0.3 is the Al content, of 5 and of 30 nm width and 225eV height. The thickness of the barrier is 20nm.

W(nm)	5			30		
	FEM (eV)	Machado (eV)	HEF (eV)	FEM (eV)	Machado (eV)	HEF (eV)
1st state	0.0722	0.075	0.0722	0.050	0.0050	0.049
2nd state				0.0199	0.0200	0.0198
3rd state				0.0446	0.045	0.0445
4th state				0.0790	0.078	0.0789
5th sate				0.1227	0.12	0.1226
6th state				0.1747	0.174	0.1745

Case 2: Layered quantum heterostructures

Fig. 3 and Table II present an example of the results obtained by QWS for an heterostructure composed by InP – 250nm, $Al_{0.175}Ga_{0.2986}InAs$ -99nm, $InGa_{0.468}As$ – 10nm, $Al_{0.175}Ga_{0.2986}InAs$ – 3nm, InAs – 9nm, InP – 250nm.

Table 2- Comparison iof the eigenvalues for a layered quantum heterostructure obtained by the two numerical methods implemented in QWS.

	HEF	FEM		
Mesh Density (points / nm)	-	5.333	10	20
1st state	0,0709	0,0697	0,0700	0,0714
2nd state	0,2855	0,2852	0,2847	0,2853
3rd state	0,3037	0,3028	0,3026	0,3037
4th state	0,4122	0,4120	0,4114	0,4118
5th state	0,4952	0,4953	0,4951	0,4950

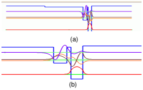


Fig. 3 (a) Quantum potential, eigenvalues and eigenfunctions for a layered heterostruture; (b) a zoom view.

Case 3: Quantum Dot Computation

The implementation of the HEF for QD was validated by comparing our results with the ones presented in (Lee et.al, 2004) for QD with three different shapes : cylinder, lens, and cone. Some results are presented in Fig. 4.

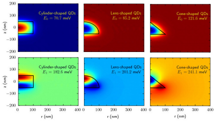


Fig. 4 - Eigenvalues and eigenfuntions for the two first bounded states in cylinder-like, lens-like, and cone-like quantum dots.

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Concluding Remarks

The first version of an 1D computer code was delivered for a basic analysis of QWIP devices. This code includes the FEM and the HEF implementations for multiquantum well. A new tool, not presented in this work, for an 1D selfconsistent computation of the quantum states was implemented and it is in testing phase.

Nowadays, the HEF has been used for the analysis of quantum dots. Moreover, an implementation of a FEM formulation, considering the axial symmetry of the problem is in testing phase. This implementation is developed using the framework of the LEVSOFT computer code, a multiphysics software based on the 2D Finite Element Method. LEVSOFT includes all the modules necessary for a complete Finite Element Analysis and presents a graphical user interface that integrate all these modules (Abe et al, 2002), (Yang et al.,2006) (Abe et al., 2006).

The software tools developed in this work are already being used in research works (Vieira et al., 2007), (Souza et al., 2007).

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