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 allow 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 and 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:

\[ -\frac{\hbar^2}{2m_e} \left[ \frac{1}{r_e} \frac{\partial}{\partial r_e} r_e \frac{\partial}{\partial r_e} \right] \psi(r_e) + V(r_e) \psi(r_e) = E \psi(r_e) \]

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

\[ \frac{h^2}{2m_e} \sum_{i,j} A_{ij} \psi_i \psi_j + \sum_{i} R_i \psi_i = E \sum_{i} N_i \psi_i \]

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

\[ \psi(r) = \sum_{i} N_i \psi_i \]

with np the number of nodal points in the finite element and \( \psi_i \) 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 C0) or of second order (quadratic base functions, with continuity C1).

A compressive 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’s 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 continuity \( C \)

\[ \frac{h^2}{2m_e} \left[ \frac{1}{r_e} \frac{\partial}{\partial r_e} r_e \frac{\partial}{\partial r_e} \right] \psi(r_e) + V(r_e) \psi(r_e) = E \psi(r_e) \]

where, \( \psi(r_e) \) is the zero of the Bessel function of order \( m \) \( J_m(k_r \rho_r) \).

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 visualization of the potential profile, eigenvalues and eigenvectors, 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 eigenvectors. 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 eigenvectors.

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 wells. A new tool, not presented in this work, for an 1D quantum well structure, is already prepared to handle both arbitrary potential and arbitrary effective mass profiles. In the present version, the computer code is limited 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 and quantum dots immersed in quantum well structures.

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., 2005). 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 and eigenfunctions for a single quantum well of effective mass \( m_r = \frac{\pi}{6} m_0 \), where \( n \) is the AO content, of 5 and of 30 nm width and 225 eV height. The thickness of the barrier is 20 nm.

<table>
<thead>
<tr>
<th>Width (nm)</th>
<th>FEM (eV)</th>
<th>Machado (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.05</td>
<td>0.05</td>
</tr>
<tr>
<td>30</td>
<td>0.12</td>
<td>0.12</td>
</tr>
</tbody>
</table>

Case 2: Layered quantum heterostructures

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.

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

<table>
<thead>
<tr>
<th>Width (nm)</th>
<th>FEM (eV)</th>
<th>HEF (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.07</td>
<td>0.07</td>
</tr>
<tr>
<td>30</td>
<td>0.41</td>
<td>0.41</td>
</tr>
</tbody>
</table>

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 eigenvectors for the two bound states in cylinder-like, lens-like, and cone-like quantum dots.

References


J. M. Machado, Y. Shiyou, J. M. Villas-Boas, G. S. Vieira et al., InAlAs/InGaAs QWIP grown on InP Substrate by MOVPE, 13 Brazilian Workshop on Semiconductor Physics, São Paulo, Brazil (2007).