

Development of Finite Element Software Tools for QWIP and QDIP Design



Roberto Yuji Tanaka, Angelo Passaro, Nancy Mieko Abe, José Maria Villas-Bôas, Gustavo Soares Vieira, Stephan Stephany (+)

Divisão de Física Aplicada, Instituto de Estudos Avancados (IEAv/CTA) - SP - Brazil

(+) Instituto Nacional de Pesquisas Espaciais (INPE) - SP - Brazil

It is service, we present a charge look and the interface of the service of the s

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 too hosed on the FEM and auviliary methods for the analysis and design of OWIP and ODI

Mathematical Formulations

The Finite Element Method (FEM)

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

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

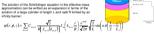
$$-\frac{\hbar^{2}}{2m}A_{ij}+(V-E)B_{ij}=0 \text{ . where } A_{ij}=\psi_{i}^{+}\left(\int\int_{\Omega}\nabla N_{i}^{*}\cdot\nabla N_{j}d\Omega\right)\psi_{j}$$

$$B_{ij}=\psi_{i}^{+}\left(\int\int_{\Omega}\nabla N_{i}^{*}\cdot\nabla N_{j}d\Omega\right)\psi_{j}$$

functions:
$$\psi(\,r\,) = \sum_{i}^{n} N_{i}(r)\,\psi_{i} \label{eq:psi_number}$$

with np the number of nodal points in the finite element and by 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 CP) or of second order (quadratic base functions, with continuity CP). A compressive evaluation of the FFM annied to the Poisson equation is presented in (Page of

The Hamiltonian Expansion Formulation (HEF)



where, $k_{n,n}$ is the n-zero of the Bessel function of order m $(J_n(k_{n,n})=0)$ The strain induced in the quartum dot due to the lattice mismatch is also taking into account

The QWS computer program

Windows graphic user interface: Lavered 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)

· Owley UED

Graphical visualisation of the potential profile, eigenvalues and eigenfunctions, Fig. 2.



quantum state. The visualization options allow putting in evidence each one of the eigenvalues

Concluding Remarks The first variation of an 1D commutate code was delivered for a basic analysis of OWIP devices. This code includes the FEM and the HEF implementations for multipusantum well. A new tool, not presented in this work, for an 1D ters on of an 1D computer code was develop to a tert computation of the quantum states was imple:

Novedays, the HEF has been used for the arehysis of quartum 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 otherwise based on the 2D Fride Element Method. LEVSOFT includes all the modules necessary for a complete Finite Element Analysis and presents a graphical user interface that imagents all these modules (and et al. 2002), (Yang et al. 2006) (Abs et al. 2 The software tools developed in this work are already being used in research works (Vieira et al., 2007). (Souza et al., 2007)

QWS Code Application

Case 1: Simple rectangular quantum well - valid

The quartum well FEM code was validated comparing our results for a single quantum well with the ones obtained in a previous work in which a meathless 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/AbcGa1-xAs rectangular quantum well, effective mass m*= (0.067 + 0.063x) m, where x = 0.3 is the Al content, of 5 and of 30 nm width and 225eV height. The thickness of the barrier is 20mm.

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

Case 2: Lavered quantum heterostructures

Fig. 3 and Table II present an example of the results obtained by QWS for an heterostructure composed by InP – 250nm, A_{0.11}Ga_{0.284}InAs – 30nm, InGa_{0.884}As – 10nm, A_{0.11}Ga_{0.884}InAs – 3nm, InIAs – 9nm, InP –





and eigenfu heterostruture: (b) a zoom view.

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.

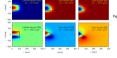


Fig. 4 - Eigenvalues and eigenfuntions for the two

N. M. Ales, A. Pessano, M.-A.P. France, F. Stotll, Y. A. Seebo, D. H. Oslar and F.J. P. Santos, Un Stalema de Software-pies Ankline de Copposition e Componentes de Cylina Heigenda, Filian Cylina e Missionnida, Avas da V. Compressi Shashoo de Estimologiecismo, Chamado (2022) Jilee, M. C.Chou, C.-S. Yang, G.J.Jan, Eigen-Energies and Eigen-Functions of Symmetroside Quantum Date, Chinese Journal of Physics, 36, 102 (00

 M. Machada, Y. Shyas, A. Passas and N.M. Ale, An Application of the Element Free Claimin Method in the Analysis of Quantum Stell Structures, Proceedings of The Fourth International Conference on Electromagnetic Field Problems & Applications - ICEP 2003, Targin, Crims, pp. 207-270 (2000) A. C. J. Parel, N. M. Alle, V. A. Sterlin and A. Passani, Simulations of Plannes with Electrociatis PIC Models Using the Finite Electron McMod, Biolites-Journal of Physios, vol.33, n.2, pp. 411417 (2002)

Y Stryou, J.M. Machado, N.M. Ale, A. Pascare, Simulation of Needle Type Control Electrodes by the Finite Element Method, Proceedings of the XVI International Conference on Class Societies and their Assistations, Xtan (China), pp. 345–365, 2006.

