Coupled Multiphysics Modeling of Semiconductor Lasers

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ABSTRACT

Comprehensive models of semiconductor lasers are required to predict realistic behavior of various laser devices for the spatially nonuniform gain that results due to current crowding. Nonuniform gain has visible effect on laser dynamics and parameters, like threshold gain. Consistent solution of coupled electrical, thermal, gain and optical problems was achieved by CFD-ACE+ integrated solver. Integration of multiphysics into a single computational environment allowed for high-efficiency, high-fidelity modeling of modern semiconductor lasers, including vertical-cavity surface-emitting lasers (VCSELs) and edge-emitting lasers (EELs).

This paper shows a full self-consistent coupling of the most-advanced-physics models of spatially dependent current flow, temperature effects, gain, and optical modes development and competition. Three coupled modules: Semiconductor Device, Thermal, and Optics, of CFD-ACE+ general purpose multiphysics software, are used in the present study.

Keywords: Semiconductor lasers, VCSELs, computational modeling

1 INTRODUCTION

CFD-ACE+ multiphysics software is an environment composed of module solvers dedicated to numerous physical areas, geometry building and meshing modules, GUI, visualization tools, data transfer facilities, optimization, computation flow and parametric run control using scripting. This environment allows to solve multiphysics problems in consistent manner. It gives great advantage over techniques using separate runs of various solvers that may lead to inconsistency and instability of solution, as well as long computation times.

The VCSEL physics includes strong nonlinear coupling of time-dependent and space-dependent optical fields, electric carriers (electron and holes) distributions in semiconductors, and temperature. Moreover multiple optical modes are coupled and energy transfers to the modes better supported by carrier concentration distribution at a given time moment. CFD-ACE+ uses an iterative

approach to solve this stiff system of equations. In the following sections we describe basic equations and methods applied in our semiconductor laser modeling software.

2 OPTICS MODELING APPROACH

Optical models include Weighted Index Method (scalar) and Method of Lines (scalar and vectorial). Both edge-emitting lasers and VCSELs can be efficiently modeled. The code allows to study transient behavior of lasers with time-dependent and spatially inhomogeneous gain. Multiple quantum wells and multiple transverse modes are included. For each time step, a calculation loop over electrical, thermal, gain, and optical solvers is performed.

2.1 VCSEL Eigenvalue Problem Solution

Solution for VCSEL transverse and axial field distribution in the modes as well as their lasing frequencies consists of solution of an eigenvalue problem for Helmholtz equation in cylindrical coordinates, and boundary value problem set by the boundary conditions at VCSEL layer and radial region interfaces.

To solve the optical eigenvalue problem for VCSEL the Weighted Index Method (WIM, [1], [2]) was applied. This method solves the Helmholtz equation for axisymmetric problem using separable eigenmode fields and harmonic azimuthal field dependence:

$$E(\rho, z, \varphi) = G(z) \cdot F(\rho) \cdot \cos(m\varphi)$$

where ρ, z, ϕ are respectively radial, axial, and azimuthal coordinates, E, G, F are electric field complex amplitudes, ω is angular frequency, c is speed of light, \mathcal{E}_r is the complex relative permittivity, and m is azimuthal mode number.

The original Helmholtz equation is replaced by two equations for axial and radial fields.

$$G''(z) + \beta_i^2 G(z) = 0$$

$$F''(\rho) + \frac{1}{\rho}F'(\rho) + [k_i^2 - \frac{m^2}{\rho^2}]F(\rho) = 0$$

where β_j , k_i are propagation constants in axial and radial direction, respectively, and indices j, i denote material layer perpendicular to optical axis, and radial region respectively.

The propagation constants β_j , k_i couple these equation. We find VCSEL linearly polarized (LP) eigenmodes by alternatively solving axial and radial constraint equations, updating weighted propagation constants, and the weighted permittivity. This iterative improvement of solutions can be understood as an enhancement of the popular effective index method.

The solutions are of the form:

$$F(\rho) = \begin{cases} c_1 J_m(k_1 \rho) \to \rho < \rho_{ox} \\ c_2 K_m(k_2 \rho) \to \rho > \rho_{ox} \end{cases}$$

$$G(z) = a_j e^{i\beta_j z} + b_j e^{-i\beta_j z} \cdot for \cdot z_{j-a} \le z \le z_j$$

where $J_m(k_1\rho)$ and $K_m(k_1\rho)$ are Bessel functions of the *m*-th order of the first kind and modified Bessel function of the *m*-th order of the second kind, ρ_{ox} is the oxide aperture radius, and a, b and c are unknown constants.

The result of the WIM analysis is a set of LP_{mn} eigenmodes (bound in radial direction and radiative in the axial direction), m is azimuthal and n is radial mode number.

The unknowns are, for each lasing eigenmode, the $F(\rho)$, G(z), the resonant frequency ω , and the imaginary part of permittivity in the active region (related to material gain)

2.2 Photon Rate Equations

For each mode, the photon rate equation is solved including optical losses, and spontaneous and stimulated emission terms taking into account spatially and time-dependent material gain:

$$\frac{dS_{\nu}}{dt} = \left(\int_{V_{QW}} R_{ST/p\nu} \, d\nu - \frac{1}{\tau_{ph}} \right) S_{\nu} + \beta_{SP\nu} \int_{V_{QW}} R_{SP} \, d\nu$$

where S_{ν} is number of photons in the mode, t is time, $R_{ST/p\nu}$ is stimulated emission rate per photon in the mode, V_{QW} is the quantum wells volume, τ_{ph} is the photon lifetime describing losses through the mirrors and absorption, R_{SP} is spontaneous emission rate, $\beta_{SP\nu}$ is a

factor describing geometrical and spectral coupling of the spontaneous emission into a mode.

Corresponding stimulated and spontaneous emission terms are responsible for carrier relaxation in the electrical model.

3 SEMICONDUCTOR MODEL

Our comprehensive laser simulation software includes a high-fidelity model of semiconductor physics, based on drift-diffusion formulation, enhanced with energy balance equations [3]. It enables a realistic modeling and simulation of VCSELs, EELs, and other optoelectronic and photonic devices.

The semiconductor physics model includes the following equations:

• Electric Potential (Poisson's) Equation

$$\nabla \cdot (-\varepsilon \nabla \phi) = q \left(p - n + N_D^+ - N_A^- \right)$$

• Carrier Continuity Equations

$$q\frac{\partial n}{\partial t} - \nabla \cdot \vec{J}_n = q(G - R)$$

$$q\frac{\partial p}{\partial t} + \nabla \cdot \vec{J}_p = q(G - R)$$

where ϕ is the electric potential, n, p - electron and hole concentrations, respectively, N_D , N_A - donor and acceptor doping concentrations, q - electron charge, ε - electric permittivity, (G-R) - generation-recombination rate, which includes Shockley-Read-Hall and Auger components.

The electron current density J_n and the hole current density J_p are:

$$\vec{J}_n = qD_n \nabla n + qn \left\{ \mu_n \nabla \left(-\phi + \frac{E_c}{q} \right) + D_n \nabla T_n - \frac{3}{2} D_n \nabla \ln m_n \right\}$$

$$\vec{J}_{p} = -qD_{p}\nabla p + qp\left\{\mu_{p}\nabla\left(-\phi + \frac{E_{v}}{q}\right) + D_{p}\nabla T_{p} - \frac{3}{2}D_{p}\nabla\ln m_{p}\right\}$$

where μ_n and μ_p are electron and hole mobilities, dependent on temperature, ionized doping density, instantaneous local carrier concentration, and electric field; T_n and T_p are electron temperature and hole temperature representing carrier energy, calculated from the equations shown below; m_n and m_p are electron and hole effective masses, respectively, and E_c and E_v are conduction and valence energy band levels.

Carrier Energy Equations

$$\frac{\partial n w_n}{\partial t} + \nabla \cdot \vec{S}_n - \nabla \left(-\phi + \frac{E_c}{q} \right) \cdot \vec{J}_n + n \frac{w_n - w_L}{\tau_{wn}} = w_n (G - R)$$

$$\frac{\partial p w_p}{\partial t} + \nabla \cdot \vec{S}_p - \nabla \left(-\phi + \frac{E_v}{q} \right) \cdot \vec{J}_p + p \frac{w_p - w_L}{\tau_{wp}} = w_p \left(G - R \right)$$

where w_n , w_p , w_L are energy densities of electrons, holes and crystal lattice, respectively. The energy fluxes of electrons and holes are

$$\vec{S}_n = -k_n \nabla T_n - \frac{1}{q} (w_n + kT_n) \vec{J}_n$$

$$\vec{S}_p = -k_p \nabla T_p + \frac{1}{q} (w_p + kT_p) \vec{J}_p$$

The above equations are solved in Semi-Device Module of CFD-ACE+ [4] in two-dimensional (2D) or three-dimensional (3D) domains, using finite-volume method (FVM). The module includes also impact-ionization model and photo-generation model for simulation of other optoelectronic devices, for example photodetectors.

4 EXAMPLE APPLICATIONS

Advanced modeling is crucial for comprehensive analysis, design, and optimization of new architectures of semiconductor lasers. One of critical problems in laser design is to avoid extensive heating of DBR due to current flow and provide uniform current flow through quantum wells. Intracavity-contacted lasers are one possibility to achieve this goal. Figure 1 shows computed current-flow vectors and electron density distribution inside an intracavity VCSEL device.

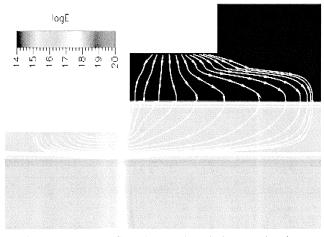


Figure 1: Current flow (vectors) and electron density distribution (colors) inside an intra-cavity VCSEL device

Figure 2 illustrates the transient behavior of multi-transverse mode operation of conventional oxide-confined VCSEL. Initially excited LP_{01} mode is after some time replaced by higher radial-order modes which are effect of higher current density close to the edge of the oxide aperture. This phenomenon is supported also by spatial hole burning in the center of the axis, and accompanied by carrier diffusion effects.

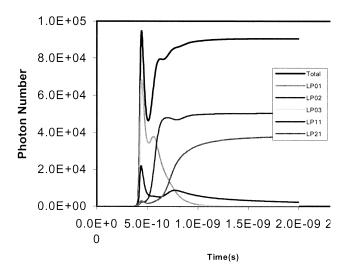


Figure 2. Transient behavior of a multi-transverse-mode VCSEL: photon numbers in particular modes and total number of photons in the cavity.

Figure 3 presents a radial distribution of intensity in particular transverse modes that were excited. To support visualization of weaker modes, each mode is normalized to have the same energy.

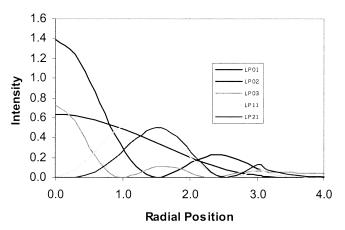


Figure 3. Steady-state radial distribution of intensity in different transverse modes for VCSEL with 6 micrometer oxide aperture.

On-axis distribution of energy in the transverse modes (with the same normalization applied) is presented in Figure 4.

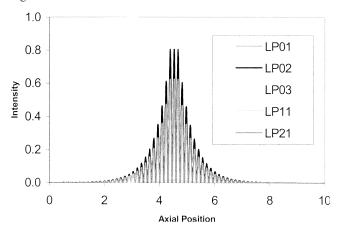


Figure 4. Steady-state axial distribution of intensity in transverse modes for VCSEL with 6 micrometer oxide aperture.

Figure 5 below is a CFD-VIEW visualization of time evolution of transverse modes in oxide confined VCSEL.

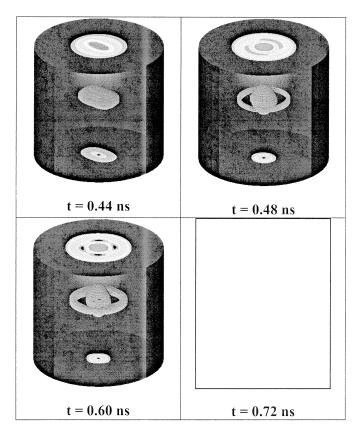


Figure 5. Selected snapshots of transient behavior of total optical intensity during the multi-transverse-mode VCSEL switching (cf. Figure 2).

5 CONCLUSIONS

A comprehensive, coupled multiphysics simulation software for semiconductor lasers has been developed and presented in this paper. CFD ACE+ solver has been used to perform transient multi-transverse mode simulation of semiconductor lasers, both VCSELs and edge-emitting devices. Solution of optical eigenvalue problem was obtained in each time step using Weighted Index Method and was consistently coupled with solutions of electric and thermal equations.

The new software is extremely fast. A Python-based scripting capability, incorporated into the computational environment, was used to obtain *I-V* and *L-I* characteristics of lasers. The code uses advanced models of refractive index and gain, dependent on multiple parameters including carrier concentration, temperature, wavelength, mole fraction, quantum well width, and waveguide width. Complex laser structures can be built, meshed, and modified using CFD-GEOM module. The Python scripting can be used to automate parametric studies of device structures. CFD-VIEW module has been used to provide data analysis and results visualization and animation.

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