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Comprehensive Simulation of Vertical Cavity Surface Emitting Lasers: Inclusion of a Many-Body Gain Model

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Abstract. This paper describes a comprehensive simulation technique for semiconductor lasers. In particular, a many-body calculation of optical gain for the quantum-well region is integrated into a multi-dimensional electro-opto-thermal simulator. Simulation results of material gain and DC device data of a commercial 850 nm Vertical Cavity Surface Emitting Lasers (VCSEL) are compared to measurements. They illustrate the validity of the approach.

Keywords: laser simulation, vertical cavity surface emitting laser, many body gain, TCAD

1. Introduction

The performance of present commercial Vertical Cavity Surface Emitting Lasers (VCSELs) is a result of carefully balancing the optical, electrical and thermal design constraints. Technology computer aided design (TCAD) supports the development process by adding to the understanding of the fundamental mechanisms as well as shortening the critical time-to-market for new or customized products. This requires simulation models that include the relevant physics in order to make predictions on novel designs using TCAD.

In this paper, an improved optical gain calculation is presented which is integrated into such a comprehensive laser simulator. The gain model is based on the semi-classical Bloch equations, and includes many-body effects. It has shown excellent agreement with experimental data [1]. This paper is organized as follows. First, the gain model is outlined, and its inclusion into the simulator is discussed. Then, comparisons to measurements from a commercial GaAs based VCSEL are made, and the results are discussed.

2. Simulation Model

The details of the opto-electro-thermal model have been described elsewhere [2,3] before. Therefore, only a brief outline is given here. The optical modes of the VCSEL microcavity are modeled by solving Maxwell's vectorial wave equation using a finite element method. Perfectly matched layer absorbing boundary conditions ensure proper treatment of radiation and diffraction effects. The interaction of the optical modes with the gain medium is based on a semi-classical description, with the classical optical field treated in the slowly varying amplitude approximation. The gain model is described in Section 3 in detail.

Carrier transport is described using a standard drift-diffusion theory, with thermionic emission currents at the hetero-interfaces. In the quantum-wells of the active region, the ballistic carrier transport is modeled with a simplified scattering equation, which balances separated bound and unbound carrier distributions [4,5]. Self-heating is treated in the thermodynamic framework, which calculates the local temperature from energy balance, assuming equilibrium of carrier and lattice temperature. The equations are solved in a self-consistent fashion applying a combination of the Newton Raphson method and and the Jacobi-Davidson QZ method in a Gummel type iteration scheme.

3. Microscopic Gain Model

Optical gain in the quantum-well region is calculated using a semi-classical approach, where gain is derived from the interaction of a classical optical field with the microscopic polarization of the charge carriers in the semiconductor. The formalism is similar to [6] and includes valence-band mixing effects, conduction band non-parabolicity, Coulomb-induced band coupling and correlation effects at the level of quantum kinetics. In contrast to [1,6], the equations are solved in a stationary mode in order to save computation time.

The microscopic polarization is obtained from its Heisenberg equation of motion. The renormalized energy is calculated with an 8-band k^*p method, and the diagonal and non-diagonal polarization dephasing rates are determined within the second Born approximation in the Markovian limit. Homogeneous broadening is calculated on a microscopic level from carrier-carrier scattering, and therefore, no heuristic broadening model is applied as for instance in free carrier theories.

The computation of a spectral gain curve with this method typically takes several hours on a high performance workstation. Therefore, it is not practical to couple the full gain calculation to a multi-dimensional laser simulator. As a solution, the spectral gain characteristics are computed prior to the device simulation, assuming flat band condition, and stored as lookup tables. The resulting material gain is stored as a function of electron and hole density, temperature and lasing wavelength. A typical gaintable, for the simulations presented in this paper, consists of different spectral curves for 15 electron densities, 15 hole densities and 15 temperatures.

The multi-dimensional electro-opto-thermal laser simulator uses a Newton method as numerical procedure. In order to include the spectral gain information into this procedure, both gain as well as its partial derivatives with respect to the system variables are needed. A finite element interpolator is applied to match the data from the gaintable to the Newton method in our case. It interpolates in the 4 dimensions electron and hole density, temperature and wavelength, and shows excellent convergence behavior when coupled to the full Newton procedure.

4. Simulation Results

The simulated device is a commercial GaAs-based single mode VCSEL emitting at around 850 nm using an oxide confinement.

In order to validate the gain model, gain measurements have been performed using a broad area (BA) edge-emitting laser with the Hakki-Paoli method. The BA laser has the same active composition as the VCSEL device, namely multiple AlGaAs quantum-wells (MQWs), In order to extract material gain from the modal gain measurements, the optical confinement factor is calculated with a finite-element method solving the vectorial Helmholtz equation. A comparison of measured and simulated gain is shown in Fig. 1 at two ambient temperatures and for different carrier densities. Excellent agreement is achieved.

The top and bottom Bragg mirrors of the VCSEL are of GaAs/AlGaAs type with approximately 30 periods each. A sketch of the simulated VCSEL device structure is illustrated in Fig. 2. In order to resolve the quarter-wavelength Bragg mirrors, the mesh for the optical solver consists of approx. 200,000 elements. The electro-thermal equations are solved on a coarser grid with approx. 20,000 elements. The material parameters are taken from literature, and are not listed explicitely due to space constraints [7].

Figure 3 shows the material gain curve extracted from the coupled 2-dimensional electro-opto-thermal simulation at different bias points. The ambient temperature is 20°C. At twice the threshold current, the maximum internal temperature is 27°C, it rises to 64°C at 3.8 times threshold current and to 102°C at 5.6 times threshold current.

The detuning between the cavity mode and spectral gain changes as well, as can be seen in the figure. Typically, the cavity mode has a redshift of 0.06 nm/K, whereas the gain peak shifts with 0.2 nm/K in this

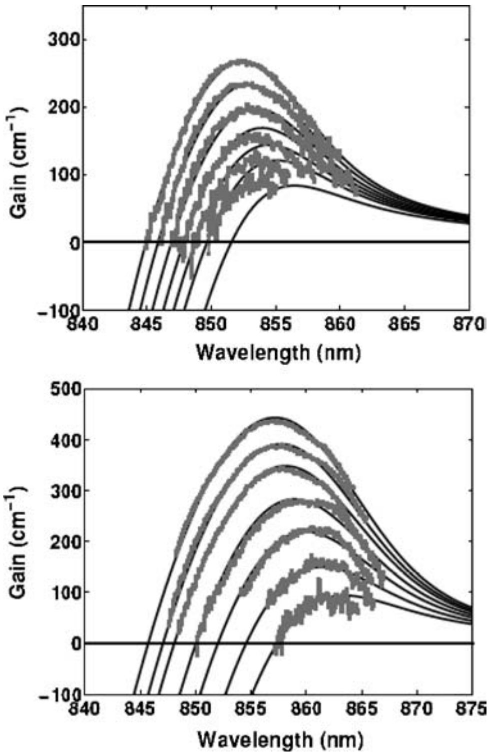

Figure 1. Comparison between measured (grey) and simulated (black) material gain for a broad area edge-emitting laser. The top curve is taken at 25°C, the bottom curve at 55°C.

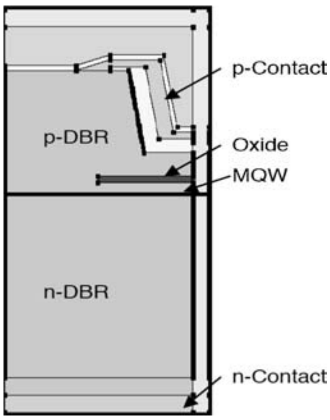

Figure 2. Schematic of the device structure used for the 2-dimensional simulation.

material system. Compared to the edge-emitter gain measurements in Fig. 1, the VCSEL has a higher threshold gain, and therefore, the material gain characteristics for higher carrier densities are needed. Accurate modeling of gain in this regime is particularly important, due to the fact that material gain is not measurable

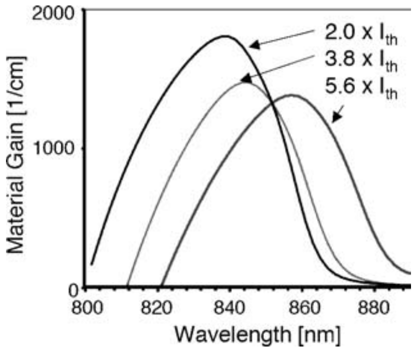

Figure 3. Simulated Material Gain in a VCSEL with an ambient temperature of 20°C under different bias currents. The lasing wavelength is approx. 851 nm. Self-heating effects change both the gain peak position and its shape with increasing current.

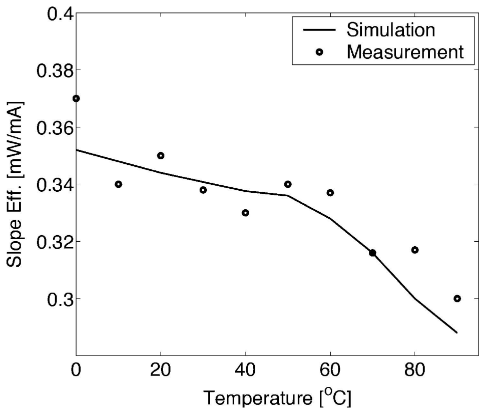

Figure 4. External efficiency versus ambient temperature. The markers show the measurements and the line is the simulation.

using standard methods in the VCSEL directly (e.g. Hakki-Paoli method).

Figure 4 shows the external efficiency of the VCSEL, both simulation and measurement. It has been assumed that the coupling efficiency in the measurement is 80%, and the resulting scaling is included in the figure. The decrease in efficiency is mainly caused by a reduction in the internal efficiency, which is impacted by thermally activated leakage currents above threshold. This is an indication that self-heating effects are modeled correctly. Rollover of the optical power versus current curve could only be observed in the multi-mode regime in the experiment. Simulation of this effect is beyond the scope of this paper.

Figure 5 shows threshold current versus ambient temperature. The u-shaped curve is typical for VCSELs and is a signature of the shift of peak gain versus cavity

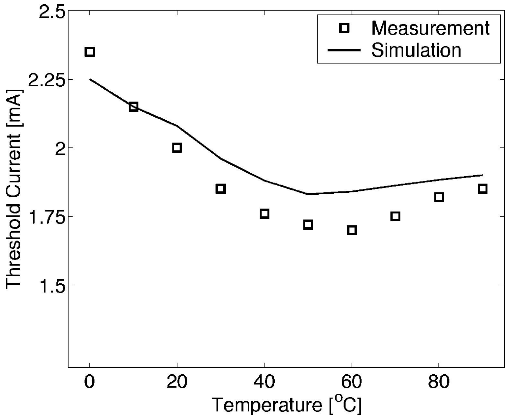

Figure 5. Threshold current versus ambient temperature. The markers show the measurements and the line is the simulation.

mode. Similar to Fig. 3, increasing the ambient temperature decreases the detuning (assuming the cavity mode wavelength is larger than the material gain peak wavelength). This in turn reduces the modal gain which is necessary to overcome the cavity loss, and therefore can lead to a situation with lower threshold currents at higher temperature. The simulation indicates that counteracting effects such as thermal broadening of the carrier distribution functions or leakage currents are less significant.

The simulation shows a less pronounced u-shape and marginally higher thresholds than the measurement. This is most likely due to a slight overestimation of a nonradiative recombination mechanism.

5. Conclusion

Inclusion of an accurate model for optical gain into a comprehensive device simulator has been presented. It is based on the semiconductor Bloch equations and treats many-body effects on a quantum kinetic level. As application, 2-dimensional simulation results of a 850 nm single mode VCSEL are in good agreement with measurements.

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7. see http://www.ioffe.ru/SVA/NSM/