Software Package for Modeling III-Nitride QW Laser Diodes and Light Emitting Devices

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Abstract: We present a modeling software package developed at Ostendo Technologies for analysis and design of semiconductor laser and light-emitting diodes. The current database of material parameters supports complete group of III-Nitride alloys used in visible spectrum applications and can be readily extended to all III-V compounds.

Keywords: Optoelectronics, laser diodes, light-emitting diodes, nitrides, III-V compounds.

1. Introduction

Nitride-based photonic devices lead the way in developing visible and UV optical range applications with electrically pumped laser diodes (LD) and light-emitting devices (LED) being in the highest demand.

Modeling of optoelectronic devices is an extremely complicated task. It involves a combination of strongly interrelated physical phenomena taking place at different space and time scales – from angstroms and picoseconds in optically active quantum wells (QW) to dc transition times and carrier diffusion lengths limited by injection and external modulation.

At least four basic software blocks or modules should be involved in full-scale LD/LED modeling and design addressing, correspondingly, the physics in microscopic active regions, the transport in the diode structure, the optical waveguiding, and the thermal management. The database of material parameters is yet another important building block of the software as illustrated in Figure 1.

In this work, we present full-scale modeling software package developed at Ostendo Technologies for analysis and design of III-V semiconductor active optoelectronic components. The current database of material parameters supports complete group of III-Nitride alloys used in visible spectrum applications and can be readily extended to all III-V compounds with corresponding extension of the spectral range of the devices [1].

2. Use of COMSOL Multiphysics

All the software components are COMSOL-based with physical models and databases originally developed at Ostendo Technologies. No specific COMSOL modules have been employed in our programs. Special effort has gone into developing the Micro module [1,2]. Self-consistent multi-band quantum-mechanical model for carrier energy spectrum in active QWs has been implemented and solved with COMSOL eigenvalue solver. Drift-diffusion equations of our Transport module are solved by nonlinear stationary solver. At this stage of development, all modeling is one-dimensional.

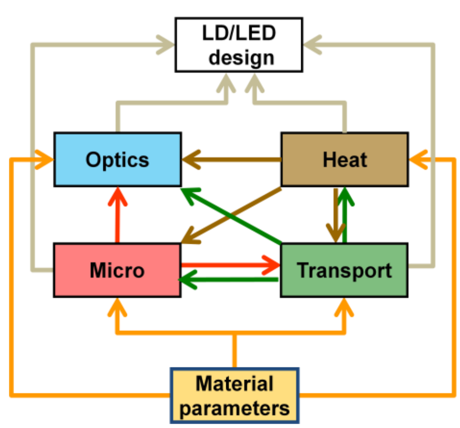

Figure 1. Flowchart of device modeling stages.

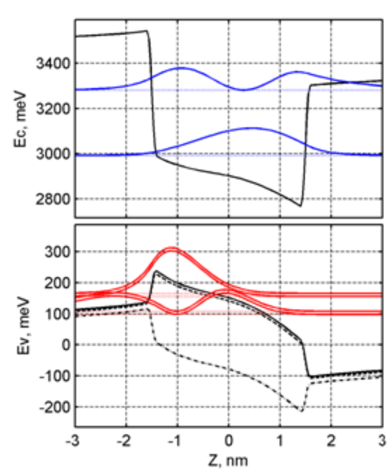

Figure 2. Band profiles and eigenstates in active QWs

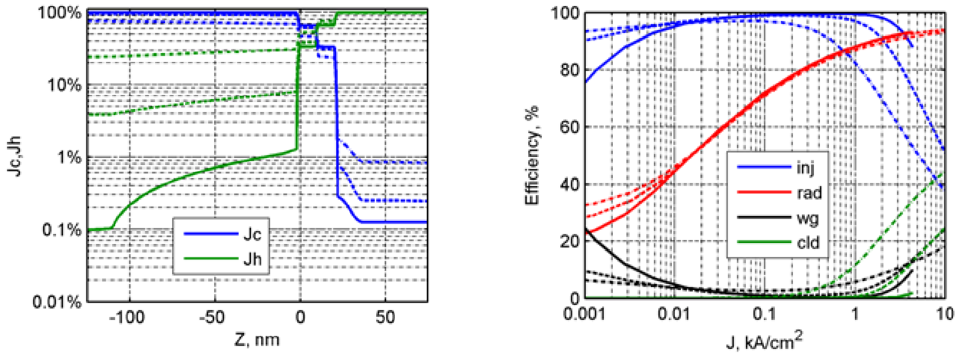

Figure 3. Injected current distribution (left) and injection, radiative, and waveguide/cladding leakage coefficients versus injection level (right) at different temperatures: solid – 300K, dash – 400K, dash-dot – 500K.

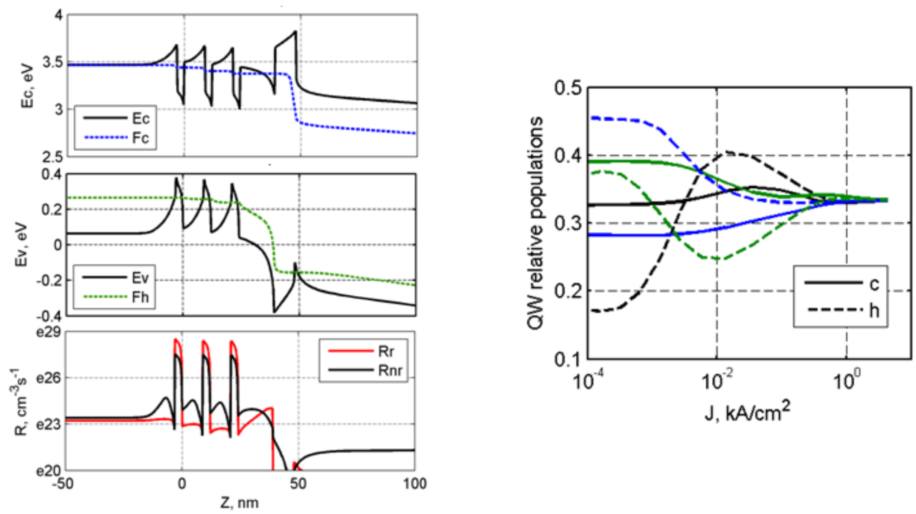

Figure 4. Band profiles and radiative/nonradiative recombination rate distribution at threshold level in three-QW structure (left); Fc/ Fh - quasi-Fermi levels. Relative QW population dynamics (right); color identifies the QW.

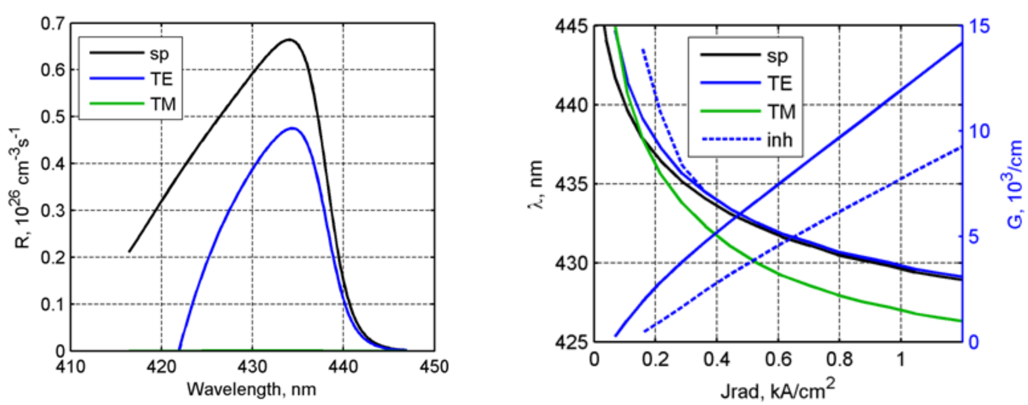

Figure 5. Left: TE gain (blue) and spontaneous emission spectra (black). Right: material gain and emission wavelength as a function of QW radiative current level; dashed lines illustrate effect of inhomogeneous broadening.

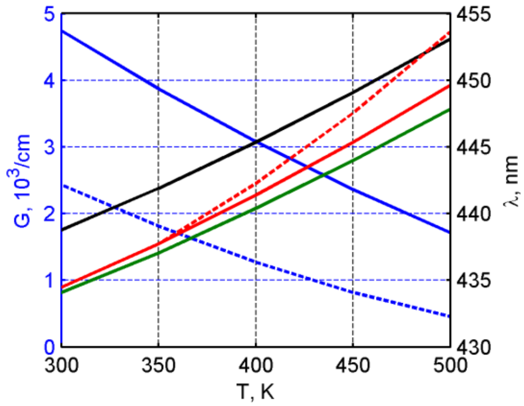

Figure 6. Temperature dependence of QW gain (blue) and emission wavelength for main transition (black), spontaneous emission (green) and peak gain (red). Dashed lines illustrate the effect of inhomogeneous broadening on peak gain and wavelength.

3. Results

The Micro module provides detailed information about microscopic structure of lasing states, allows calculation of electron and hole energy spectra and modeling of QW optical characteristics. Module output includes: (1) self-consistent band profiles including strain effect, spontaneous- and piezo-polarization; (2) QW subband dispersions with band-mixing and nonparabolicity; (3) confined energy levels and subband DOS; (4) optical matrix elements and optical anisotropy coefficients; (5) emission wavelength shift with injection; (6) carrier statistical distribution and subband populations; (7) spontaneous and stimulated emission rates; (8) optical gain spectra, peak optical gain, and induced refractive index change; (9) differential optical gain (with respect to concentration and radiative current); (10) transparency concentration level and corresponding radiative current.

The Transport module provides distribution of injected carriers and corresponding recombination rates throughout the structure as a function of injection current. Module output includes: (1) self-consistent band profiles and charge carrier distributions in active region; (2) injected current distribution; (3) radiative and nonradiative recombination rate distributions; (4) relative QW populations; (5) free-carrier absorption distribution; (6) I-V characteristics; (7) injection and radiative efficiency; (8) leakage current.

The Optical module provides transverse optical mode distribution and estimation of modal refractive index. Module output includes: (1) refractive index profile at lasing wavelength and modal refractive index; (2) transverse optical mode distribution; (3) QW optical confinement factors.

At this level of program development the heat management has not been yet independently addressed. In all modules, temperature effects are treated parametrically. Self-heating effect estimation is based on the experimentally determined structure thermo-impedance

The Final design module combines the results obtained in the Micro, Transport, and Optical modules. The final design module is based on phenomenological characteristics approximating the more detailed results of each particular module, like efficiency parameters, gain coefficients, confinement and loss factors, etc.

Module output includes: (1) L-I characteristics; (2) threshold current and characteristic temperature; (3) differential quantum (slope) efficiency and characteristic temperature; (4) output optical power and wall-plug efficiency; (5) dependence of threshold and efficiency on the emission wavelength; (6) dependence of LD threshold and efficiency on the total number of QWs.

Input/Output interface programs generate modeling log file automatically assembling tables of calculated parameters and figures of modeled device characteristics.

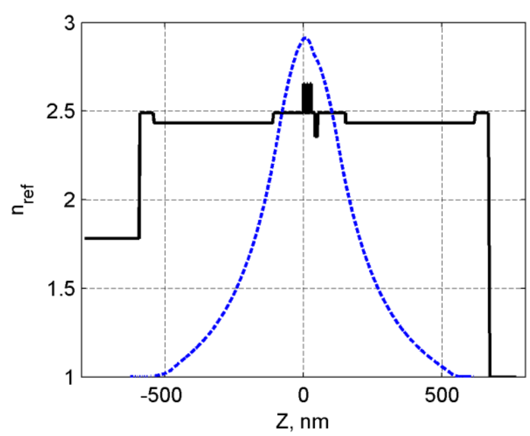

Figure 7. Refractive index and main optical mode profile for 3-QW LD structure on sapphire substrate.

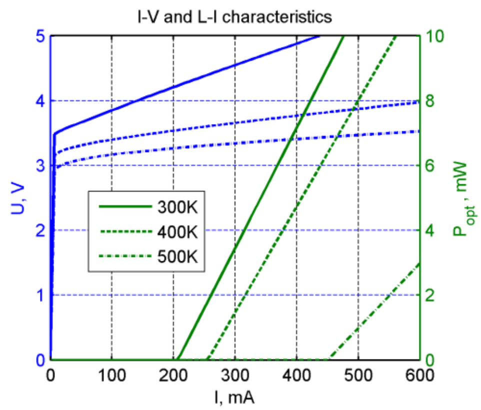

Figure 8. L-I-V characteristics of 3-QW LD structure at different temperatures.

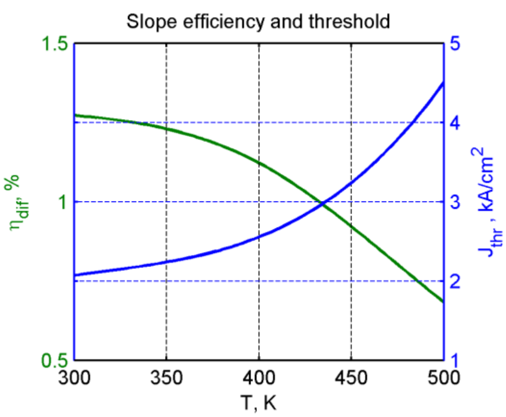

Figure 9. Temperature dependence of differential quantum efficiency and threshold current density.

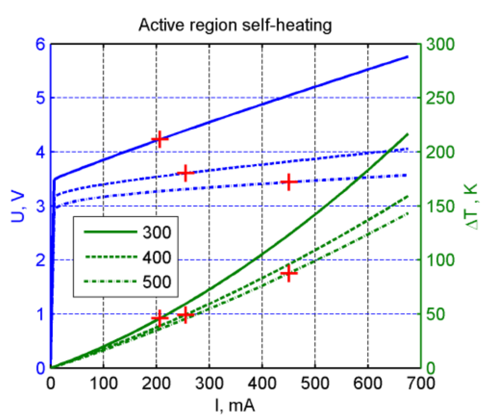

Figure 10. Active region temperature rise for DC laser operation. Red crosses mark the threshold values.

4. Exemplary calculation

We illustrate the software capability by modeling a typical blue-range laser diode with symmetrical optical waveguide layout comprising active region with three 3 nm wide GaInN QWs. Figures 2-10 exemplify the design process and illustrate the main characteristics of the structure.

5. Conclusions

Development of physics-based modeling tools with open access to the model contents utilizing COMSOL Multiphysics is the most efficient way to design elaborate contemporary optoelectronic devices based on novel physical principles and/or new material systems. COMSOL Multiphysics make possible creating flexible and yet comprehensive physical models which facilitate the design even for the most untraditional devices. We provide a brief description of full-scale modeling tools developed at Ostendo Technologies, Inc. for design of III-Nitride based active optoelectronic devices. Already, using this COMSOL-based software package we have made useful observations on the design and performance of GaInN laser diodes [3, 4].

6. References

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