Simulation of Quantum Cascade Lasers

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Contents

- Microscopic rate equation approach
- Challenge in carrier transport modeling
- Solution in 2/3D simulator
Subband engineering

Given MQW structure, all quantum states are solved.

Energy levels and intersubband transition dipole moments computed for all pairs of states.

Critical states identified according to design ideas such as the so-called 3-level design.
Simulation procedures

- Set up 1D mesh for two periods of QCL in gain-preview session.
- Assume a uniform applied field and solve the quantum states.
- Discretize Schrödinger equation in 1D and solve with sparse eigen matrix techniques.
- Identify and label states belonging to injection or active regions, based on shape and location of wave functions and their respective energy levels.
Microscopic rate equations

- Equations in form: \( \frac{dn}{dt} = \frac{n}{\tau_{in}} - \frac{n}{\tau_{out}} \).
- Coupled with cavity photon rate equation.
- Relate device current to injection region current.
- Closed set of equations to get lasing characteristics.
Electron distribution based on subband population calculated by microscopic rate equations
First 9 levels are plotted with the first three levels in active region labeled.
Increasing current from 10 to 500 mA with peak gain set by threshold at 150 mA.

All possible intersubband transitions evaluated assuming wavelength independent waveguide loss and broadening constant.
Reasonable agreement with experiment achieved.
Two injection schemes

(a) Assume all tau’s are constants and all levels are initially unoccupied. Current injection increases occupancy until lasing.

(b) Assume injection region and active level1 are initially occupied. 1/tau_injection set to increase linearly with current to preserve total sheet charge.
Remarks

• Stimulated recombination in QC laser does not pin the carrier density but only levels it off. Overall densities in active region still increase substantially as current is injected.

• Lack of density pinning explains absence of lasing relaxation oscillation in laser turn-on/off.

• Lasing action does not require or imply charge neutrality.
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Challenges in transport modeling

- **Microscopic rate equations:**
  - Time constants contain no information on how electrons get there from the contacts.
  - One still has to work on transport on larger size scale.
Challenges in transport modeling

- **Commonly used device simulators:**
  - Mobility-based drift-diffusion and thermionic emission.
  - Quantum tunneling done for few barriers as correction to drift-diffusion model.

- **Requirement for QCL:**
  - Drift-diffusion and thermionic emission still needed.
  - Quantum tunneling for hundreds of barriers.
Going beyond quasi-equilibrium?

High field

Conventional Fermi-Dirac

Tunneling emitter src

Transport may not be local or sequential
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Equations and models

- The conventional:
  - Drift-diffusion equations with thermionic boundary.
  - Scalar optical mode solver.
  - Laser cavity photon rate equation.

- QCL specifics:
  - Local optical gain as a function of local current according to microscopic rate: $g(J,S)$.
  - Within period: transport between injection/active regions according to microscopic rate eq.
  - Non-local transport between periods and to/from contacts.

Resonant tunneling effects
Non-local injection model

Between periods

To/from contacts

Injection with mean free path
Non-local injection mobility

Increase of mobility due to build-up of hot carriers and lowering of tunneling barriers at higher fields.
QCL 2D example

25 periods, assuming same MQW and microscopic rates as in previous sections.
Optical mode

Wave_Intensity 1

+Y

1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
2
4
6
8
10
12
14
+X

Wave_Intensity 1

0
0.2
0.4
0.6
0.8
1.0
Current distribution

- $J_y$ (A/cm$^2$)
- $\log_{10}(J_x)$
Band diagrams (QCL 25 periods)

0 Volt

2.5 Volt

5 Volt

10 Volt
1D cuts of electron concentration and Jy (@10 V)

Reduction caused by current spreading
Rem: a single mode does not use all the periods.

Much stronger gain suppression than LD

Non-linear gain suppression
I-V and modal gain spectrum

Remark: turn-on voltage sensitive to field dependence of non-local injection mobility ➔ May not have a classical interpretation.

Remark: change in shape indicates non-linear suppression.

Modal gain at 0, 2.5, 5, 7.5 and 10 volts.
Lasing characteristics and efficiency per period

Yet to be included:
1) Heating effect.
2) Gain peak detuning due to potential variation.

Source of inefficiency:
1) Lack of overlap with single mode.
2) Nonradiative transition within microscopic rate model.
3) Part of non-local current excluded from the microscopic rate model.
Summary

- Subband structure calculation enables the basic design of QCL such as emission wavelength and miniband alignments.

- Microscopic rate equation model generates a convenient optical gain as a function of local current and photon densities $g(J,S)$.

- Main challenge in macroscopic QCL simulation is to inject electrons from contact to MQW and to collect them from MQW to contact.

- We propose a non-local current injection model with a mean-free-path of 100 -1000 Å.

- Field dependent mobility of non-local injection needed to obtain reasonable results.
About Crosslight

- A leading semiconductor TCAD provider since 1993
- Complete product portfolio for semiconductor device simulation
- Innovative simulation tools to ensure a fast and seamlessly transfer from process to device simulation
- Ultra efficient 3D structure combined with powerful and easy to use 3D editor to provide class leading 3D simulation experience
- “Café-time Simulator”. Windows based, user friendly graphic user interface makes simulation more enjoyable.