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Modeling of mid-infrared quantum cascade lasers: The role of temperature and operating field strength on the laser performance

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ABSTRACT

In this paper a self-consistent numerical approach to study the temperature and bias dependent characteristics of mid-infrared (mid-IR) quantum cascade lasers (QCLs) is presented which integrates a number of quantum mechanical models. The field-dependent laser parameters including the non-radiative scattering times, the detuning and energy levels, the escape activation energy, the backfilling excitation energy and dipole moment of the optical transition are calculated for a wide range of applied electric fields by a self-consistent solution of Schrodinger–Poisson equations. A detailed analysis of performance of the obtained structure is carried out within a self-consistent solution of the subband population rate equations coupled with carrier coherent transport equations through the sequential resonant tunneling, by taking into account the temperature and bias dependency of the relevant parameters. Furthermore, the heat transfer equation is included in order to calculate the carrier temperature inside the active region levels. This leads to a compact predictive model to analyze the temperature and electric field dependent characteristics of the mid-IR QCLs such as the light-current (*L–I*), electric field-current (*F–I*) and core temperature-electric field (*T–F*) curves. For a typical mid-IR QCL, a good agreement was found between the simulated temperature-dependent *L–I* characteristic and experimental data, which confirms validity of the model. It is found that the main characteristics of the device such as output power and turn-on delay time are degraded by interplay between the temperature and Stark effects.

1. Introduction

Quantum cascade lasers (QCLs) [1] are high-performance mid-infrared (mid-IR) light sources based on resonant tunneling (RT) and intersubband transitions (ISTs) of electrons in quantum wells. In contrast with conventional semiconductor lasers based on interband transitions, in which the emission characteristics are affected by the energy bandgap, in QCLs the emission wavelength is mainly determined by the proper choice of barrier and well layers thickness. The cascading scheme and unipolarity are other characteristic features of QCLs that make this kind of device so unique. The active material of a QCL typically contains a cascade of many, more than ten, pairs of active regions and injectors including tens of interfaces. In general, the active region transport is controlled by ultrafast ISTs and typically requires a bias of several hundred mV per module at threshold for laser action. Compared with bipolar semiconductor lasers, QCLs suffer from large threshold current and voltages which lead to strong local heating effects inside the device active region [2]. Because of the positive feedback loop between increasing laser core temperature and threshold current density, the device active region can be at a considerably higher temperature than the heat sink which affects the device optical gain [3,4]. Several temperature-activated processes have been suggested to cause the degradation of the laser gain with temperature: (1) escape of thermally activated electrons from the upper laser state into higher energy continuum-like states, (2) thermal backfilling of electrons from the downstream electron reservoir into the lower laser state, (3) reduce of the laser upper state lifetime by the Bose factor at higher temperatures, (4) decreases of the stimulated gain cross section with temperature, and (5) increase of the waveguide losses with temperature [5–7]. Another important aspect about the degradation of laser gain is the Stark-effect rollover, which is the common problem with QCLs far above threshold. In QCLs, Stark-effect is due to an increases in voltage across the device, which causes a misalignment between the ground state of injector and the upper laser state in the active region. This in turn, results in a loss of injection into the upper laser state, and conductive path for electrons from the injector into the continuum-like states above the wells and barriers [8]. These factors combine to reduce the population inversion between the upper and lower laser states and, hence, the laser gain decreases.

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Clearly, to gain a deeper understanding in the QCL design, the development of a simple and reliable simulation model which account for the thermal and bias dependence of a QCL's behavior is a necessary prerequisite. To investigate and understand the underlying physical process for a general QCL structures, there are several useful approaches, such as self-consistent rate equations model [9,10], the Monte Carlo simulation [11], the density matrix methods [12,13], the hybrid density-matrix Monte Carlo model [14], and the quantum theories based on nonequilibrium Green's function [15,16] have been developed. While these modeling approaches are accurate, the implementation of such models is difficult and their computational are very demanding. Recently, a number of transport models based on the density matrix formalism [17,18] have been developed, capable to estimate actual laser performance, i.e., the output power and the voltage-current characteristic. While these models are simpler and faster than their highly numerical alternatives, they are limited to steady simulation, and they still require a description of thermal-dependent mechanisms in the QCL.

In this paper, we extend the theoretical model of previous works [19,20] and develop a self-consistent numerical approach by employing a number of optoelectronic models including: the Schrodinger–Poisson equations to compute the quantization states, longitudinal optical (LO) phonon scattering time, detuning and excitation/activation energies, and dipole moment of the optical transition; the carrier coherent transport with sequential resonant tunneling to adopt the electric field-current (*F*–*I*) relationship in the device; the simplified four-level rate-equation model to describe the carrier and photon dynamics inside the active region levels; and the heat transfer equation to incorporate the heat dissipation. Furthermore, we focus on understanding electron pathways in the band structure of mid-IR QCLs to elucidate the factors that limit the operation of the device in presence of temperature and electric field.

This paper is organized as follows. In Section 2, the corresponding self-consistent numerical approach consisting of band structure calculation, the combination of carrier coherent transport with a simplified four-level rate equations as well as the heat transfer equation are introduced. Section 3 discusses the numerical implementation of the model. In Section 4, the numerical results are carried out for a given structure. In Section 5, we bring the conclusions.

2. Theoretical model

2.1. Electronic structure

The subband wavefunctions $\psi_n(x)$ and igenenergies E_n are determined by the Schrodinger-Poisson system [21],

$$\left[-\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{m^*(E,x)}\frac{d}{dx}+V(x)-E_n\right]\psi_n(x)=0, \tag{1}$$

$$-\varepsilon\frac{d^2\phi(x)}{dx^2}-q\left(N_D(x)-\sum_n n_{2D,n}\left|\psi_n(x)\right|^2\right)=0, \tag{2}$$

where q and $\hbar$ respectively are the electronic charge and the reduced Plank constant, $m^*(E,x)$ is the spatial and energy dependent effective mass, which includes the nonparabolicity coefficient, $N_D(x)$ is the doping concentration of the structure, ε is the position dependent permittivity and $n_{2D,n}$ is the electron sheet density of level n, due to the doping concentration. The self-consistent potential is given by $V(x)=V_0(x)-q\varphi(x)$, where $V_0(x)$ is the conduction band profile and $\varphi(x)$ is the electric potential due to the space charge profile.

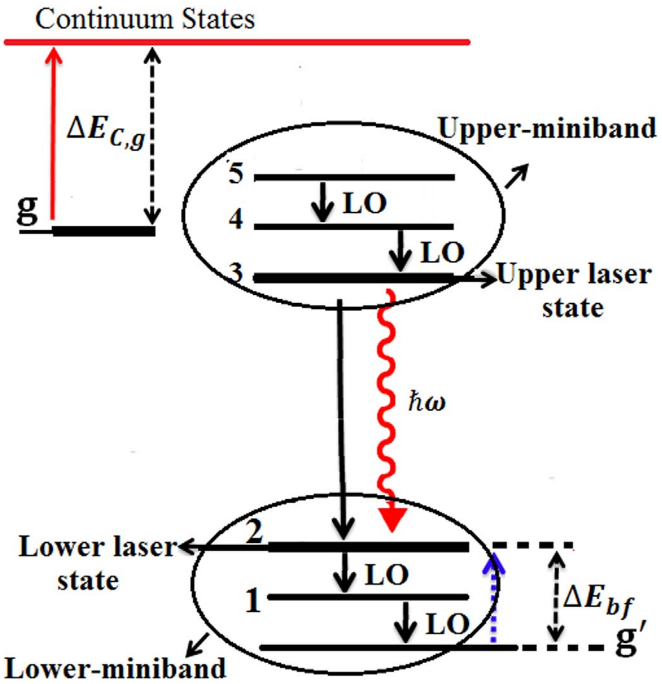

Fig. 1. Schematic representation of a mid-IR QCL-active region with the various relaxation processes indicated by arrows.

In ISTs, the lifetimes of the energy levels are mostly affected by the nonradiative scattering mechanisms such as impurity, interface roughness, electron-electron, acoustic phonon and LO-phonon scattering process. In the mid-IR QCLs, where energy levels spaced by more than one optical phonon energy, the LO-phonon scattering is the dominant process [22], and we take into account only this process based on Ferreira and Bastard's approach [23]. In the following, to compute the dipole matrix element of the optical transition, we adopt the formulation described in [24], in which we consider the influence of the valence band part of the wavefunctions.

2.2. Carrier coherent transport in QCLs

A schematic representation of the dynamical processes occurring within a general QCL active-region is given in Fig. 1. It is well known that the active region of mid-IR QCLs operates under a strong electrical bias, which breaks the upper laser miniband of the superlattice into a set of localized state (labeled as 3, 4 and 5 in Fig. 1). In the QC laser, carrier transport is controlled by ultrafast ISTs between the quantized states and carrier injection is accomplished by RT of electrons from the injector ground state g into the excited state 3 [25]. The RT occurs when two energy states (the states g and 3) anticross across the injection barrier at a given electric field. After the anticrossing, a further increase in the field misaligns these two states and the device enters a region of negative differential resistance (NDR). As the bias is increased furthermore, the injector ground state is brought in resonance with the other states 4 and 5, sequentially, and creates the current path for the device in parallel with the injection into the state 3 [25]. According to density matrix theory, taking into account of the second-order contribution to tunneling which caused by the difference between the populations of electrons in both sides of injection barrier [26], the current density between the injector ground state g and the laser upper state $i(=3, 4, 5)$ can be

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