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Self-consistent electro-opto-thermal model of quantum cascade lasers with coupled electron and phonon interactions far from equilibrium

Hossein Reza Yousefvand

Department of Electrical Engineering, Islamshahr Branch, Islamic Azad University, Tehran, 33147-67653, Iran

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ABSTRACT

A self-consistent model of quantum cascade lasers (QCLs) is presented here for the study of the QCL's behavior in the far from equilibrium conditions. The approach is developed by employing a number of physics-based models such as the carrier and photon rate equations, the energy balance equation, the heat transfer equation and a simplified rate equation for the creation and annihilation of nonequilibrium optical phonons. The temperature dependency of the relevant physical effects such as stimulated gain cross section, longitudinal optical (LO) phonons and hot-phonon generation rates are included in the model. Using the presented model, the static and transient device characteristics are calculated and analyzed for a wide range of heat sink temperatures. Besides the output characteristics, this model also provides a way to study the hot-phonon dynamics in the device, and to explore the electron temperature and thermal roll-over in the QCLs.

1. Introduction

Quantum cascade lasers (QCLs) are mid-to-far infrared unipolar semiconductor devices based on intersubband transitions (ISTs) between quantized states within the conduction band [1]. In a system with reduced dimensionality such as the QCL, emission of optical phonon is the dominant process controlling the electronic transport and ISTs in the device active region [2]. This ultrafast nonradiative process makes the carrier lifetime in the upper laser state very short, on the order of magnitude 10^{-12} s. Consequently, the typical threshold currents in QCLs are much larger than is common for conventional diode lasers, with their much longer carrier lifetimes, on the order of a few nanoseconds due to the nature of spontaneous and band-to-band Auger recombination processes [3]. In QCLs, the interaction of electrons and optical phonons plays a central role in our understanding of the electronic transport and optical properties of the device.

During typical QCL operation, electrons in the active region will be accelerated and hence gain a large amount of kinetic energy. These energetic electrons are often referred to as hot electrons; because the characteristic temperature of these electrons will be much higher than that of the surrounding crystal lattice [4,5]. Electrons release this excess energy by exciting other electrons and emitting photons or phonons. Due to the requirement of conservation of energy and momentum during the hot electron relaxation process, the longitudinal optical (LO) phonons that created in this way will have a certain distribution in momentum space; thereby phonons with different wave vectors may have different occupancies, so they are often called hot phonons or nonequilibrium phonons [4]. Another important aspect about the generated LO-phonon is that the nonequilibrium LO-phonon decay into two short wavelength longitudinal acoustic (LA) phonons, which this process is often referred to as anharmonic decay [6]. Anharmonic decay rate is typically an order of magnitude slower than their LO-phonon generation, so QCL operation is accompanied by a considerable accumulation of nonequilibrium phonons [7]. In the other word, unbalance between phonon generation and phonon annihilation may produce a nonequilibrium population of optical phonons. The presence of a hot phonon population significantly affects electronic transport and electron cooling rate, thereby influencing optical gain and laser threshold. Therefore, the electron–phonon interaction has to be modified substantially to account for the hot-electron and hot-phonon effects.

However, to gain a deeper understanding of physical processes within a QCL active region, the development of a systematic and compact theoretical model that account for hot-electron and hot-phonon dynamics is a necessary prerequisite.

In this paper we present a self-consistent approach which integrates the relevant interaction mechanisms such as the electrical, optical and thermal properties in QCLs. The model is developed by employing a number of standard physics-based approaches including: a simplified two-level rate equations to describe the carrier and photon dynamics in the active region levels; the energy balance equation to adopt the electron temperature in the upper and lower laser states; the heat

E-mail address: hossein@iiau.ac.ir.

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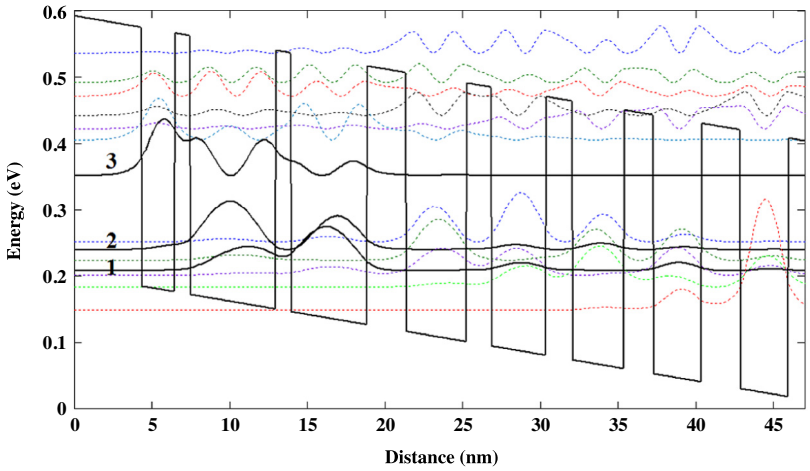

Fig. 1. Self-consistent computation of the energy band diagram and moduli squared of the wave functions for one period of the understudy QCL. The sequence of layer thicknesses in nanometers, (from left to right) starting from the injector barrier, is: /**4.5**/2/**1.1**/5.4/**1.1**/4.8/**2.6**/3.8/**1.7**/3.4/ **1.8**/3.2/**2**/3/**2.6**/3. $Al_{0.45}Ga_{0.55}As$-barrier layers are in bold, and GaAs-well layers are in regular, and doped layers ($n = 4 \times 10^{17}$ cm^{-3}) are underlined.

transfer equation to calculate the lattice temperature; and a simplified non-equilibrium phonon's rate to account the hot phonon dynamics. The coupled equations are solved self-consistently in the transient and steady-state conditions for a wide range of sink temperatures (200–320 K). The results of these calculations can then be used to achieve the output characteristics, and to explore the hot phonon dynamics and electron temperature. The paper is organized as follows: in Section 2, we discuss about the physical model used to analyze the QCLs, including: the bandstructure calculation, description of the thermal, carrier and photon dynamics within the device active region, as well as we discuss about the nonequilibrium electron–phonon interactions. In Section 3, the numerical results are carried out, with focusing on the static and dynamic operation conditions. Finally, in Section 4, we bring the conclusions.

2. Physics and theory

2.1. The QCL bandstructure

In this work, we investigate a GaAs-based lattice matched $Al_{0.45}Ga_{0.55}As$/GaAs mid-infrared (MIR) QCL [8] with a laser cavity area of 20 μm × 3 mm. For one period of the structure, the subband energies and wave functions are calculated by a self-consistent solution of Schroedinger–Poisson system with conduction band dispersion nonparabolicity. Fig. 1 gives the calculated electrical potential and relevant squared wave functions for each subband in the active region under a bias electric field of 40 KV/cm. In order to facilitate system-level design and output characteristic simulation, a simplified schematic representation of the relevant dynamical processes occurring within the active region, i.e., the energy dynamics, the thermal dynamics and the carrier dynamics, is illustrated in Fig. 2.

2.2. Thermal dynamics in QCLs

It is well established that the active region of QCLs operates under a strong applied electric field. With high-intensity fields, large amounts of energy are pumped into the electronic system, thereby electrons will be accelerated and gain a large amount of kinetic energy, which relax by transferring much of it to the lattice as the phonon. These energetic electrons are often referred to as hot electrons; because if we assume that they reach a thermal equilibrium among themselves, then the characteristic temperature of these electrons will be much higher than that of the surrounding crystal lattice [4,5]. The kinetic energy of two-dimensional electrons can be characterized by an effective temperature T_E, which is moreover the same in both the upper and lower laser states.

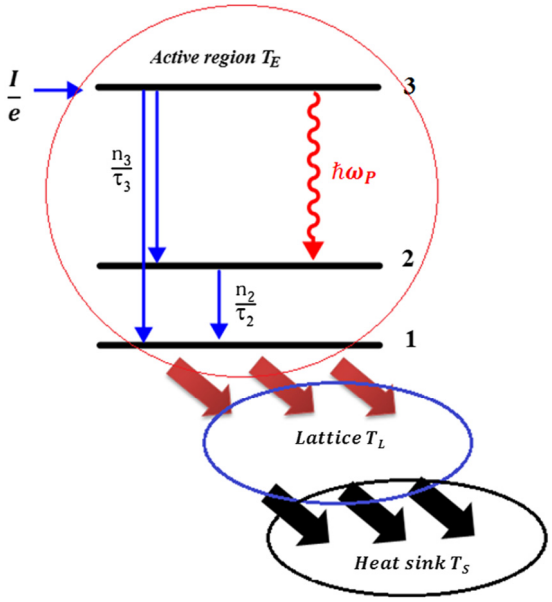

Fig. 2. Simplified dynamic diagram of the relevant interaction mechanisms occurring within the QCL, i.e., the energy dynamics, the electron dynamics as well as the thermal dynamics.

The experimental and theoretical works [9,10], justify the use of an average electron temperature for both the upper and lower laser states, with a good approximation in MIR QCLs. In this case, one should also consistently take into account the dependence of the electron cooling rate due to the stimulated photon emission. Therefore, gain or loss of the total energy of the two-dimensional electrons in the active region can be modeled via a simple rate equation as previously done in [11,12]:

$$n_{2D}K_B\frac{dT_E}{dt} = \frac{I}{eA}\left(\Delta E_{3,2} + \Delta_{2,g}\right) - n_{2D}K_B\frac{T_E - T_L}{\tau_E} - G_P(n_3 - n_2)N_p\hbar\omega_p \quad (1)$$

where I is the total current flowing through the device, e is the electronic charge, n_{2D} is the surface doping concentration per stage, K_B is the Boltzmann constant, $\Delta E_{3,2}$ is the energy difference between the upper and lower laser states, $\Delta_{2,g}$ is the energy difference between the lower laser state and injector ground state of the next stage, T_L is the lattice temperature, τ_E (= 0.22 − 0.25 ps) is the energy loss lifetime between the electronic and lattice temperature. Furthermore, G_P is the optical gain,