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The generation rate of optical phonons in quantum cascade lasers under different applied field

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ABSTRACT

We have theoretically studied the generation rate of longitudinal optical (LO) phonons in mid-infrared quantum cascade laser so as to learn the effect of phonons on electron transmission characteristics. The LO phonon performance was analyzed by combining the Monte-Carlo simulation with kinetic equations. We have obtained the LO phonon number under different applied field to show that the generating rate and the saturating number of optical phonon increases with applied field. At last we propose the pulsed pumping to point out the importance of LO phonon decaying into two acoustic phonons in electron transmission.

1. Introduction

Since the invention in 1994 [1], quantum cascade laser (QCL) has been proved to be one of the most effective means to generate laser radiation used for the mid-infrared optical detecting. It has also been making dramatic progress in high device performance at room temperature (300 K) [2,3]. As a complex quantum system, QCL can be modeled in various ways such as the rate equation model [4,5], Monte-Carlo (MC) simulation [6–9], and the non-equilibrium Green's function with the density matrix model [10,11]. The rate equation method in the design of mid-infrared QCLs cannot take fully into account of the complexity of temperature and density which mainly depend on the scattering time. However, by the MC method, we can intentionally turn on and off each mechanism to study its influence on the electron transport property of the device.

In our simulation, we take into account the electron-electron (e-e) and electron-LO phonon (e-LO) scattering and neglect the interface roughness and the carrier-impurity scattering as these processes do not change the trend of current-voltage [6]. It is well known that LO phonon emission exhibits a weak temperature dependence on transitions between states with an energy separation around or larger than the phonon energy [12]. For e-e scattering, we employ the single subband static screening model, and only take into account the interaction between electrons in the same or neighbor modules in one period. Only the Γ-valley states are included in the simulation, as it has been demonstrated that inter-valley leakage in this. particular QCL design is negligible [13]. For the LO phonon decaying into acoustic phonons process, we introduce the relaxation time τ_{ph} and our simulation time interval is much smaller than it [14,15].

In semiconductor heterostructures and the related devices, if the excess energy supplied to the electronic ensemble is sufficiently high, the process of electron cooling will generate non-equilibrium optical phonons which, in turn, will cause substantial changes of the carrier relaxation [16]. The energy relaxation of carriers is determined mostly by electron-LO phonon interaction and it has been shown that the phonon population decreases leading to the lattice temperature increases [17]. An electric current flowing through a semiconductor can produce coherent acoustic and optical phonons via the Cerenkov Effect as long as the electron drift velocity exceeds the phonon phase velocity [18]. Following three requirements are required for practical use of the Cerenkov Effect: high electron mobility, large electron density, and strong coupling between electrons and amplified phonons. Advanced technology of semiconductor heterostructures allows one to manipulate electron and phonon properties and makes it possible to employ the Cerenkov Effect on optical phonon generation rate. The confinement of electrons and optical phonons within the same quantum well provides the necessary strong coupling [19].

The impact of nonequilibrium LO phonon on the electronic

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relaxation dynamics and the performance of QCLs had been addressed theoretically in the past [14,19–21]. Nonradiative recombination process tends to limit the high-temperature performance of mid-infrared lasers. Phonon reabsorption, however, changes the occupation probability and influences the threshold conditions [22], the LO phonons scattering dominate the characteristic of carriers' transportation. Former experimental and theoretical studies have pointed out the distinctive nonequilibrium phonon features both in mid-infrared and THz QCLs [23,24], evidencing a significant heating of both the electronic and lattice systems. While phonons and carriers phase coherence effects have been investigated at the ultrafast timescale [25], they are expected to play a minor role in the steady state regime. Lots of phonons as the continuous voltage pumping generates contributing to the electron and lattice temperature and will hinder the electron cooling in room temperature performance, we propose the periodic pulsed voltage pumping to reduce the electronic thermal effects in the end. In the process we focus on the LO phonon lose process and decaying into acoustic modes after the voltage is removed.

2. Theory frame

Our MC model follows a conventional scheme of an ensemble of particle. We concentrate on the LO phonon performance in two steps: generating and decaying. The process of electron cooling generates a significant nonequilibrium optical phonon population that may cause substantial changes in the carrier relaxation kinetics in the semiconductor systems [8–10]. The energy dissipation has two steps: the carrier subsystem transfers a significant amount of energy to the quasi-particle (LO phonon) one; the latter, in turn, will transfer its excess energy to additional degrees of freedom and decay into two acoustic phonons [9–12]. The description of the coupled phonon nonequilibrium dynamics in prototypical mid-infrared emitting QCL can be performed within a pure semi-classical picture, in which the relevant kinetic variables are electron and phonon distributions. Then the carrier distribution function and its scattering dynamics can be parameterized by a real-space coordinate. But such non-homogeneities are characterized by a space scale which is much longer than the carrier coherence length [13–18]. The electron eigen state and energy band profile are obtained by solving the Schrödinger-Poisson equations [15,20,26]. We simulate the quantum multi-wells structure mid-IR QCL from Ref.9 with the Boltzmann transport equation (BTE) to describe the carrier and phonon coupled equations:

$$\frac{df_{vk}}{dt} = \left.\frac{df_{vk}}{dt}\right|_{e-LO} + \left.\frac{df_{vk}}{dt}\right|_{e-e} \tag{1a}$$

$$\frac{dN_q}{dt} = \left.\frac{dN_q}{dt}\right|_{e-LO} - \frac{N_q - N_0}{\tau_{ph}} \tag{1b}$$

where $f_{v,k}$ is the electron distribution function corresponding to the single-particle state in subband v and with in-plane wave vector $\boldsymbol{k}$, N_q is the average phonon occupation number which is pertinent to a single LO phonon mode with wave vector $\boldsymbol{q}$. τ_{ph} is the decay time constant of LO phonon. Many theoretical and experimental works have been carried out to determine the lifetime of the LO phonon, which shows that LO in bulk GaAs is between 3.5 and 10 ps. Actually, it is not easy to obtain a very precise value of LO phonon lifetime in GaAs-based QCLs [14,15]. Consequently, we use the assumed τ_{ph}=8.5 ps in our calculations [9]. $N_0=1/[\exp(\hbar\omega_{LO}/k_bT_L)-1]$ is the Bose-Einstein distribution of phonons at the lattice temperature T_L, $\hbar$ is the reduced Planck constant, $\hbar\omega_{LO}$ =36 meV is the assumed LO phonon energy, k_b is the Boltzmann constant. The equations are coupled through the electron-phonon collision integrals, which can be evaluated using Fermi's Golden Rule and periodic boundary conditions[6]:

$$\left.\frac{df_{vk}}{dt}\right|_{e-LO} = \sum_{q\pm}\left(N_q + \frac{1}{2} \pm \frac{1}{2}\right)\sum_{v'k'}\left[(1-f_{vk})P^{q\pm}_{vk,v'k'} - (1-f_{v'k'})P^{q\pm}_{v'k',vk}\right] \tag{2}$$

$$P^{q\pm}_{vk,v'k'} = \frac{2\pi}{\hbar}\left|g^{\pm}_{vk,v'k';q}\right|^2 \delta(\varepsilon_{vk} - \varepsilon_{v'k'} \pm \varepsilon_q) \tag{3}$$

$g^{\pm}_{vk,v'k';q}$ are matrix elements of the electron-LO phonon coupling coefficients. δ function means the kinetic energy conservation, ε refers to the state energy.

We derive a general formula of the phonon population N_q as a function of time via the Cerenkov Effect with the kinetic conservation equation [18]:

$$\frac{dN_q}{dt} = \gamma_q^{(+)}(1+N_q) - \gamma_q^{(-)}N_q - \beta_q N_q \tag{4}$$

where $\gamma_q^{(\pm)}$ are parameters determining the evolution of N_q with time due to the interaction with electrons, the updated electron-phonon scattering rate is proportional to N_q for phonon absorption $(-)$ and to N_q+1 for emission $(+)$. $\beta_q=(0.8\sim1.2)\times10^{11}\ s^{-1}$ is an estimated constant parameter to describe the phonons loss rate. When we remove the voltage there is only β_q left with hot phonons. The probabilities of the emission and absorption of phonons by the electrons can be calculated from the electron-phonon interaction using the MC simulation with the coupled BTE. We get the LO phonon number from Eq. (4) and add it into the Eq. (1a).

In Eq. (4), we represent the term associated with stimulated processes as: $\left(\gamma_q^+ - \gamma_q^-\right)N_q = \gamma_q N_q$.

And the parameters for the kinetic equation in the form:

$$\gamma_{q,m}^{(\pm)} = \frac{4e^2m^*\omega_{LO}\left(1/\kappa_\infty - 1/\kappa_0\right)G_m^2}{\hbar^2L|q|[\kappa_{el}(q,\omega_{LO})]^2\left[q^2 + \left(\frac{\pi m}{L}\right)^2\right]}\Gamma^{(\pm)}(q) \tag{5}$$

where e is the electric charge, κ_∞ and κ_0 are high and low frequency dielectric constant of the crystal respectively. m is the discrete (transverse) number of confined LO phonon and $G_m=8/[\pi m(m^2-4)]$. L=60 nm is the period length of injection and active region. In order to get the optimized value of γ_q, we set the m=1 as The value of γ is maximal for the lowest optical mode with m=1 [18]. κ_{el} $(q,\ \omega_{LO})\approx1$is the estimated electron permittivity depending on the LO phonon wave vector $\boldsymbol{q}$ and frequency, we get the simplified value:

$$\gamma_q^{(\pm)} = \left(\frac{8}{3\pi}\right)^2\frac{4e^2m^*\omega_{LO}\left(1/\kappa_\infty - 1/\kappa_0\right)}{\hbar^2L|q|\left[q^2 + \left(\frac{\pi}{L}\right)^2\right]}\Gamma^{(\pm)}(q) \tag{6}$$

In our n-doped AlGaAs/GaAs heterostructure, κ_0=12.9, and κ_∞=10.8, $m^*=0.067m_0$ is the effective mass, where m_0 is the mass of free electron. Finally the factors $\Gamma^{(\pm)}$ are:

$$\Gamma^{(\pm)}(q) = \frac{2\pi^{3/2}n}{k_0\sqrt{\Xi}}\exp\left[-\frac{1}{4\Xi}\left(\frac{k_0}{q} + \frac{q}{k_0} - 2\Omega\right)\right] \tag{7}$$

where $\Xi=k_bT_e/\hbar\omega_{LO}$, $\Omega=m^*V_{dr}/\hbar k_0$, $k_0=\sqrt{2m^*\hbar\omega_{LO}}/\hbar$, k_b is the Boltzmann constant, T_e is the electronic temperature, n is the electron concentration, V_{dr} refers to the mean drift velocity of electrons. Here we set $n=3\times10^{12}\ cm^{-2}$, $q=2\times10^6\ cm^{-1}$. As a function of the electric field, T_e is estimated from the energy and momentum conservation equations. We present the function of γ with V_{dr}, as shown in Fig. 1, γ depends on V_{dr} strongly: increasing