Role of interface roughness in the transport and lasing characteristics of quantum-cascade lasers

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A density-matrix based theory of transport and lasing in quantum-cascade lasers reveals that large disparity between luminescent linewidth and broadening of the tunneling transition changes the design guidelines to favor strong coupling between injector and upper laser level. This conclusion is supported by the experimental evidence.
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The past decade has seen spectacular progress in the development of quantum-cascade lasers (QCLs) which since their inception in 1990s[1] have been spectacular as the QCLs evolved from a scientific curiosity into practical devices producing watt-level infrared radiation at room temperature for variety of applications.[2,3] QCLs have also been a subject of extensive theoretical and modeling work, which for the most part relied upon extensive (e.g., Monte Carlo) numerical simulations.[4] Moreover, it is remarkable that all this recent success in experimental implementation of QCLs has been accomplished with quite limited theoretical input, and to this date most of successful QCL devices incorporate[5] essentially the same design principles developed in 1990s,[6,7] that in turn have relied heavily on the very first steps in understanding of the physical processes in the intersubband lasers made in 1970.[8]

Fundamentally, one period of a QCL (Fig. 1) incorporates an active region with an upper (ul) and lower lasing (ll) levels and one or more "dumping" levels separated from the lower laser level by a few phonon energies[9] to assure quick depopulation of ll. Alternatively, the ll and the dumping layers can be very closely spaced and then one ends up with a confined-to-continuum scheme.[10] Also incorporated in each period is the injector serving to quickly move the electrons into the ul of the next period. The transport through the injector is of mixed resonant and phonon-assisted tunneling nature but the last vital step of the transition from the lowest injector level (i) to the ul occurs via resonant tunneling.

The choice of the coupling between injector and ul is so critical because on one hand, large coupling energy $\hbar\Omega_c$ is required to maintain high current and quickly populate ul but on the other hand, when the coupling becomes too large, one essentially ends up with two coupled states spanning across both injector and active regions that are split by $2\hbar\Omega_c$, which gravely affects the laser gain shape and magnitude. According to the widely accepted theory of Kazarinov and Suris,[8] the resonant current density can be written as

$$J = eN_s \frac{2\Omega_c^2 \tau_\perp}{1 + \delta_{iu}^2 \tau_\perp^2 + 4\Omega_c^2 \tau_{u\to l}\tau_\perp}, \quad (1)$$

where N_s is doping density per period, δ_{iu} is the detuning of tunneling transition, $\tau_{u\to l}$ is the ul lifetime, and $\tau_\perp$ is the momentum relaxation time in the quantum well plane, usually related to the in-plane mobility. This time is also responsible for the broadening of the laser gain[3] and luminescence. Based on Eq. (1), it is desirable to have coupling strong enough that the maximum current is determined only by τ_{ul}, i.e., $\Omega_c \gg (\tau_{\mathrm{ul}}\tau_\perp)^{-1/2}$,[7] yet the coupling should not exceed the gain broadening to avoid the splitting of gain in two; hence, one must maintain $\Omega_c \ll \tau_\perp^{-1}$. This tradeoff yields optimized $\Omega_c \sim \tau_{u\to l}^{-1/4}\tau_\perp^{-3/4}$, which for typical values of $\hbar\tau_\perp^{-1} \sim 10$ and $\hbar\tau_{u\to l}^{-1} \sim 0.3$ meV yields desired splitting between two coupled levels $2\hbar\Omega_c \leq 10$ meV as is indeed done in most successful designs.

The original approach[8] did not specify the origin of in-plane momentum relaxation (broadening) which was assumed to be equal for all transitions, optical, or tunneling ones. But in the mid-IR QCLs the main origin of broadening is interface roughness[11] and it is well known that different

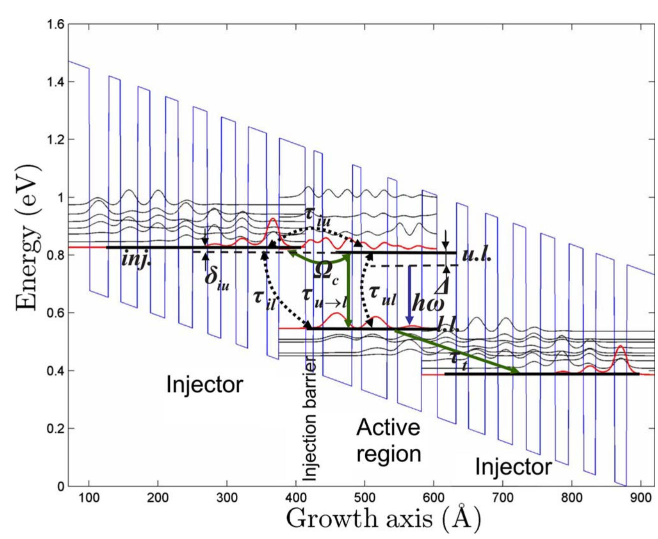

FIG. 1. (Color online) Energy diagram of a 4.7 μm QCL with relevant transition times indicated by the solid arrows and dephasing times indicate by the dashed arrows.

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transitions see different broadenings. The interface roughness broadening of the transition between two levels described by the envelope wave functions $\varphi_m(z)$ and $\varphi_n(z)$ can be written as[11,12]

$$\hbar\tau_{m,n}^{-1} = \frac{2\sqrt{2\pi}}{3}\frac{\pi m_c}{\hbar^2}\Delta_h^2\Lambda^2\left\{\sum_i \delta U^2(z_i)[\varphi_n^2(z_i)-\varphi_m^2(z_i)]\right\}^2, \tag{2}$$

where $\delta U(z_i)$ is the band offset at ith interface and the interface roughness height is characterized by mean square roughness Δ_h and correlation length Λ. Thus in QCL of Fig. 1, the broadening (dephasing) of vertical lasing transition $\hbar\tau_{\mathrm{ul}}^{-1}$ where both levels are localized in the active region is substantially lower than the broadening of diagonal transition $\hbar\tau_{il}^{-1}$ (Ref. 12) and tunneling transition $\hbar\tau_{iu}^{-1}$, where two states are localized in different regions. The width of lasing transition can be obtained from the luminescence measurements—then the widths of all other transition can be found by scaling using Eq. (2) and we indeed obtain quite different FWHM broadenings $2\hbar\tau_{\mathrm{ul}}^{-1}\sim 21$, $2\hbar\tau_{iu}^{-1}\sim 98$, and $2\hbar\tau_{il}^{-1}\sim 66$ meV, which are all in turn much broader than the lifetime broadening $\hbar\tau_{u\to l}^{-1}<1$ meV. These disparities are of great consequence to the QCL design.

To fully understand it we have solved the complete density-matrix equation for the three-level system of Fig. 1, in which tunneling characterized by coupling strength $\hbar\Omega_c$ and optical transitions caused by laser field of intensity I_l occur simultaneously,

$$\frac{d}{dt}\begin{pmatrix}\rho_{ii} & \rho_{iu} & \rho_{il}\\ \rho_{ui} & \rho_{uu} & \rho_{\mathrm{ul}}\\ \rho_{li} & \rho_{lu} & \rho_{\mathrm{ll}}\end{pmatrix} = j\left[\begin{pmatrix}\rho_{ii} & \rho_{iu} & \rho_{il}\\ \rho_{ui} & \rho_{uu} & \rho_{\mathrm{ul}}\\ \rho_{li} & \rho_{lu} & \rho_{\mathrm{ll}}\end{pmatrix},\begin{pmatrix}\delta_{iu} & \Omega_c & 0\\ \Omega_c & 0 & \Omega_l\cos\omega t\\ 0 & \Omega_l\cos\omega t & -(\omega-\Delta)\end{pmatrix}\right] - \begin{pmatrix}-\beta^{-1}\rho_{\mathrm{ll}}\tau_t^{-1} & \rho_{iu}\tau_{iu}^{-1} & \rho_{il}\tau_{il}^{-1}\\ \rho_{ui}\tau_{iu}^{-1} & \rho_{uu}\tau_{u\to l}^{-1} & \rho_{\mathrm{ul}}\tau_{\mathrm{ul}}^{-1}\\ \rho_{li}\tau_{il}^{-1} & \rho_{lu}\tau_{\mathrm{ul}}^{-1} & \rho_{\mathrm{ll}}\tau_t^{-1}-\beta\rho_{uu}\tau_{u\to l}^{-1}\end{pmatrix}, \tag{3}$$

where Δ is detuning of transition frequency ω_{ul} from optical field frequency ω, lasing Rabi frequency is $\hbar\Omega_l=(2\eta_0 e^2 z_{\mathrm{ul}}^2 I_l/n)^{1/2}$, $\eta_0=377\ \Omega$, z_{ul}^2 is the dipole matrix element, τ_t is the effective injector transport time, and $\beta(T)<1$ is the lower laser state thermal backfilling parameter. Using the latter two parameters allows us to avoid explicit incorporating in the density-matrix equation all the injector levels except the last one.

Proceeding with a standard steady-state solution, we can obtain the expression for the steady-state gain coefficient $\gamma=8\pi\alpha_0 N_s z_{\mathrm{ul}}^2\omega/\Omega_l dn\times\mathrm{Im}(\rho_{\mathrm{ul}}e^{-j\omega t})$, where d is the thickness of one period of QCL, n is the refractive index, and α_0 is a fine structure constant. For the case of laser being at or near threshold $\Omega_l\sim 0$, we obtain

$$\gamma = \gamma_0\frac{2\Omega_c^2\tau_{iu}\tau_p}{1+\delta_{iu}^2\tau_{iu}^2+2\Omega_c^2\tau_{iu}\tau_p}\times\frac{[1+\Delta^2\tau_{il}^2+\Omega_c^2\tau_{il}\tau_{\mathrm{ul}}]+\dfrac{\tau_{il}(1+\delta_{iu}^2\tau_{iu}^2)}{\tau_{u\to l}-\beta\tau_t}[1+(\Omega_c^2-\Delta^2)\tau_{il}\tau_{\mathrm{ul}}]}{[1+(\Omega_c^2-\Delta^2)\tau_{il}\tau_{\mathrm{ul}}]^2+\Delta^2[\tau_{il}+\tau_{\mathrm{ul}}]^2}, \tag{4}$$

where $\tau_p=2\tau_{u\to l}+\tau_t$ is the minimum pass time through one period $\gamma_0=4\pi\alpha_0 z_{\mathrm{ul}}^2\omega\tau_{\mathrm{ul}}N_s(\tau_{u\to l}-\beta\tau_t)/\tau_p dn$ is the maximum gain. The first term in Eq. (4) characterizes the resonant tunneling current dependence on voltage (via δ_{iu}). In contrast to Eq. (1), it contains a very short dephasing time τ_{iu} associated with localization in different regions, rather than much longer laser transition dephasing time τ_{ul} that is measured in luminescence experiments. Furthermore, gain saturation depends not just on ul lifetime $\tau_{u\to l}$ but also on the transport time τ_t of injector. Hence maximizing of current calls for $\Omega_c\gg(\tau_{iu}\tau_p)^{-1/2}$. The width of resonant tunneling peak (nearly 100 meV) indicates that rather than exhibiting negative differential resistance (NDR), the current in QCL should simply saturate as is indeed the case in most experiments. One can easily interpret the absence of NDR region as the result of localization.[13]

The second term in Eq. (4) characterizes the line shape and it has two components. The first component represents the splitting of the upper laser level due to coupling with injector which becomes observable only when $\Omega_c\sim(\tau_{\mathrm{ul}}\tau_{il})^{-1/2}$, i.e., with considerably stronger coupling than what one would expect based on the linewidth of lasing transition τ_{ul}^{-1} obtained from the luminescence or absorption measurements. The second component of the numerator in Eq. (4) represents stimulated coherent transfer of population directly from the injector to the lower laser level—one can think of this process as a stimulated Raman process in which the role of the pump is played by tunneling current. Since the upper level lifetime $\tau_{i\to u}$ is at least an order of magnitude longer than the dephasing time τ_{il}, the coherent term plays a very small role and presents mostly an academic interest for the Mid IR QCLs but in far IR devices where both dephasing

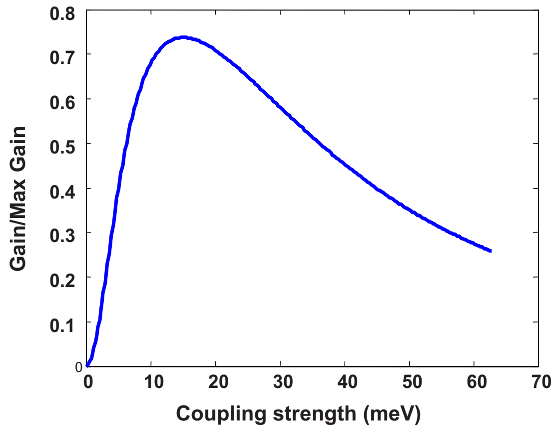

FIG. 2. (Color online) The gain coefficient as a function of energy level splitting $2\hbar\Omega_c$ in QCL of Fig. 1.

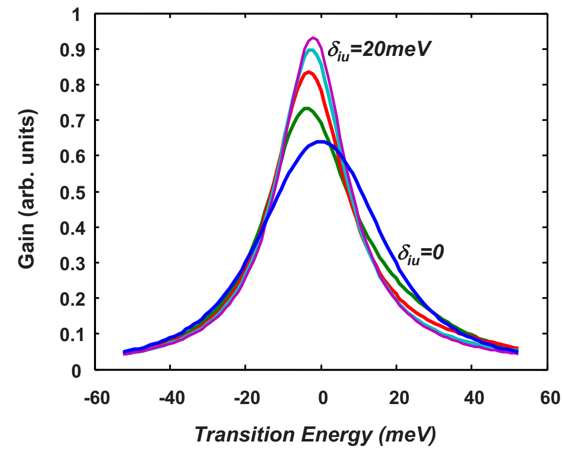

FIG. 3. (Color online) The shape of laser linewidth for different detuning between injector and upper laser level.

and depopulation have the same phonon scattering origin the coherent contribution may be noticeable.

The plot of gain versus coupling strength Eq. (4) versus for $\Delta=0$ and $\tau_t \sim 2$ ps (estimated as the time for emission of successive six optical phonons[3]) is shown in Fig. 2 and exhibits a steep rise followed by a rather gentle fall off and simple optimization show that the maximum is reached when $2\hbar\Omega_c \sim \hbar(\tau_p \tau_{iu} \tau_{il} \tau_{\mathrm{ul}})^{-1/4}$, i.e., it is essentially a geometric mean of all the broadenings in the system. For a typical mid-IR QCL of Fig. 1 with parameters mentioned above, it yields optimal splitting of 18 meV. When the QCL with newly optimized splitting had been fabricated, it has indeed shown excellent maximum current and low temperature wall-plug efficiency of up to 34%.[14]

It is worthwhile to point out that the large (factor of 3) disparity of dephasing times τ_{ul} and τ_{il} leads to an interesting phenomenon of the line shape of gain (and luminescence) broadening rather splitting into two due to coupling between injector and upper level. This is simply the result of upper laser level wave function spreading into the injector region, where it is affected by the roughness that is completely uncorrelated with roughness of the lower laser level—hence less of "subtraction" in Eq. (2) takes place and the apparent linewidth widens to more or less geometric mean $(\tau_{\mathrm{ul}} \tau_{il})^{-1/2}$. One may compare this phenomenon with the tunneling induced transparency—equivalent of electromagnetically induced transparency (EIT) first observed in intersubband transitions in Ref. 15 when the effective linewidth of a relatively broad transition had been narrowed due to admixing of a very narrow transition. Thus here we are dealing with the exact opposite of EIT. As the tunneling resonance is detuned the linewidth returns to the original narrow linewidth τ_{ul}^{-1} of decoupled transition as shown in Fig. 3 and has been indeed observed in Ref. 11.

In conclusion, we have developed a rigorous density-matrix model for current and gain in QCL that takes into account the disparity between different dephasing times cause by interface roughness. Using the theory, we have shown that the coupling between injector and upper laser level should be much stronger than previously accepted values. These conclusions had been verified experimentally.

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