Effects of interface roughness scattering on device performance of indirectly pumped terahertz quantum cascade lasers

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Abstract. The impacts of interface roughness (IR) scattering on device performance of indirectly-pumped (IDP) terahertz quantum cascade lasers are studied. Three different active region designs with almost the same lasing frequency at threshold and comparable oscillator strength are experimentally investigated and the measurement data are analyzed and compared with numerical simulation. The simulation results show that all structures suffer from the detrimental effect of intersubband roughness scattering in terms of threshold current density, and probably operating temperature. The intrasubband IR scattering time could also to be a limiting factor in the IDP structures due to the employed high energetic barrier.

1. Introduction
After more than one decade of the invention of first terahertz (THz) quantum cascade laser (QCL) [1], this device has not satisfied the basic requirement of most of industrial applications for room temperature operation. Even though different design schemes were theoretically studied and some of them experimentally implemented, none of them could operate without an inconvenient cryogenic cooling system. In 2012, Fathololoumi et al. [2] presented a structure based on resonant-phonon (RP) scheme and improved the operating temperature of THz QCLs to ∼ 200 K. The oscillator strength study on three-well RP-QCLs showed that any further improvement in this design scheme needs detailed understanding of carrier transport in THz QCLs [3]. The tall barrier study in the hope of decreasing the leakage currents in the RP structures could only lead to some minimal device performance improvements [4].

A drawback of the RP structure is the fundamental limit of less than 50% population inversion [5, 6, 7, 8]. To overcome this limitation, the indirectly-pumped (IDP) scheme, originally implemented by Yamanishi in mid-infrared (MIR) QCLs [9], emerged to be a good candidate for high operating temperature applications. Kumar et al. [6], Fujita et al. [10], and Dupont et al. [8], proposed different IDP schemes based on different material systems, while the best performance was achieved by Kumar et al. with a structure that lased up to 163 K at 1.8 THz (k_BT/ħω = 1.9). Contrary to the first two structures that employed a resonant tunneling followed by a phonon relaxation transition to depopulate carriers from the lower lasing state, Dupont et al. used a direct phonon relaxation transition, also called phonon-phonon-phonon (3P)
scheme, in order to avoid the broadening of gain induced by the resonant tunneling. Shortly after that, two different structures based on the 3P scheme were implemented with different figures of merit but the same material system, however the improvement in operating temperature was not as good as expected [11, 12]. In this paper, we investigate how interface roughness scattering affects the device performance of 3P based THz QCLs. In the 3P structures, since both injection of carriers to the upper lasing state (ULS) and their depopulation from the lower lasing state (LLS) are mediated by phonon relaxation transition, the voltage drop of each module is higher than that of conventional RP structures. This enforces to increase the energetic barrier height (from 15% aluminum composition in conventional RP structures to 25% in the 3P structures) in order to reduce electron leakage to the continuum band. On the other hand, a higher energetic barrier introduces more IR scattering, which could significantly degrade the device performance. To quantitatively investigate the IR effects on the different parameters of each structure, we selected three of our 3P-QCLs that have almost the same lasing frequency, number of modules in the active region, and doping concentration per module. The similarity in the lasing frequency at threshold and the doping concentration roughly ensure a same cavity loss among the selected three structures.

2. Effect of IR scattering on effective lifetime
The three QCL structures under study are named after their wafer numbers, respectively. V845 [11] and V895 are four-well structures with three-dimensional doping concentration of $9 \times 10^{15} \text{cm}^{-3}$ while V962 [12] is a five-well structure with three-dimensional doping concentration of $7.6 \times 10^{15} \text{cm}^{-3}$. Since the MBE growth and the fabrication process of all

Figure 1. a) Schematic diagram of a 3P-QCL active region based on a phonon-photon-phonon configuration. The solid lines show the forward scatterings, while the dashed lines show the back scatterings. $\Delta$ and $\Omega$ are the detuning and the coupling between states 1 and 4, respectively. The green arrows represent the correct injection and extraction, while the red arrows represent the wrong injection and extraction in each module. b) Conduction band diagram and the moduli squared wavefunctions of the THz 3P-QCL, V895, at 21 kV/cm. The quantum wells and barriers of V895, starting with the injector barrier, are $44/66.85/12.55/88.95/25.55/73.4/3.45/94$ Å in thickness, where the bold font indicates the Al$_{0.25}$Ga$_{0.75}$As barriers. The center of the injector barrier was delta-doped with Si to $3.67 \times 10^{10} \text{cm}^{-2}$.
presented structures were done in a similar manner, it is reasonable to assume that they have the same growth and waveguide quality. The detail of quantum design and physical processes of V845 and V962 were discussed in [11] and [12], respectively. We analyze the design structure and carrier transport of the 3P structure by presenting the schematic design scheme and conduction band diagram of V895 in Figure 1. Levels 1, 2, 3, and 4 are the ground state (also called the extraction state), the lower lasing state, the upper lasing state, and the upper phonon state (also called the injection state) of the structure, respectively. Electrons, tunneling from level 1' to the level 4, will be injected to the level 3 (ULS) via a phonon scattering relaxation mechanism. The lasing transition occurs between the levels 3 and 2. Due to sub-picosecond scattering time of 4 → 3 and 2 → 1 transitions, the current density of the structure is largely regulated by tunneling time (1' → 4) and the scattering time between the lasing state (3 → 2). At low temperatures, the scattering time between the levels 3 and 2 before the threshold electric field is mainly attributed to the interface roughness scattering time [13]. The energy spacing between those states is less than 15 meV for all three structures which results in a phonon scattering time of more than 10 ps at 50 K. In addition, the impurity scattering time between the lasing states at low temperature is also more than 20 ps for all 3P-QCLs. The effective lifetime (\(\tau_{\text{eff}}\)), interface roughness scattering time (\(\tau_{\text{IR}}\)), and total scattering time between the lasing states (\(\tau_{32}\)) were calculated based on the model presented in [8]. The expression of effective lifetime, which links population inversion with current density, when including the effect of 2 → 3 backscattering, reads as:

\[
\tau_{\text{eff}} = \frac{g_{43}(g_2 - g_{32}) - g_{42}(g_3 - g_{23})}{g_4(g_3g_{21} + g_{23}g_{31})},
\]

Figure 2. Different scattering times between the lasing states (level 3 and 2) of devices V845 (dashed red lines), V895 (dashed black lines), and V962 (solid blue line) at lattice temperature of 50 K. The electronic temperature in all subbands was assumed at 100 K.
where $g_{ij}$ is the scattering rate from state $i$ to state $j$ and $g_i$ is the total intersubband scattering from state $i$. IR scattering was identically applied on both types of interfaces: well-on-barrier and barrier-on-well with the parameters $\Delta = 0.28$ nm for the mean height of roughness and $\Lambda = 6.5$ nm for the correlation length. These times are plotted as a function of electric field in Figure 2. It shows that all three structures have an IR scattering time of less than 4 ps at threshold, which strongly affects the total scattering time between the lasing states and consequently, the effective carrier lifetime. From Figure 2, the effective lifetime of these devices at their threshold electric field at 50 K are extracted; their values vary considerably, i.e., 1.1 ps in V845, 0.72 ps in V895 and 0.61 ps in V962. Extensive variations are also observed in threshold current density at 50 K: 0.89 kA/cm$^2$ in V845, 1.33 kA/cm$^2$ in V895 and 1.47 kA/cm$^2$ in V962. It clearly shows that a higher threshold current density is associated with a shorter effective lifetime. This can be explained as following. Considering the fact that the gain of the structure will be pinned to the cavity loss at threshold point, the product of threshold current density, the effective lifetime, inverse of superperiod, and the oscillator strength of these three structures should remain roughly constant if we assume that the product between cavity loss and gain bandwidth scales with the inverse of IR-limited effective lifetime, and also, to illustrate this hypothesis graphically, we defined a function $LB$ (in THz.cm$^{-1}$) versus electric field ($E$):

$$LB(E) = 43.72 \times f_{23}(E) \times \tau_{\text{eff}}(E) \times J_{\text{th,exp}}/L_p,$$

(2)

where 43.72 is a constant value ($10^{-12}e/2\pi m_{0}\epsilon_{0}nc$) that depends on the effective mass, the permittivity of the material and the speed of light, $\tau_{\text{eff}}$ is given in ps, $J_{\text{th,exp}}$ in A/cm$^2$, $L_p$ is the superperiod in Angstrom. Figure 3 represents the calculated $LB$ as a function of electric field for the three structures. The three $LB$ values at threshold electric field, marked by square dots, are reasonably comparable among the three structures, confirming a constant cavity loss-bandwidth product of these devices. The small variation of the $LB$ values of the marked dots in Figure 3 (ranging from $\sim$36 to $\sim$39 THz.cm$^{-1}$) may come from an uncertainty in gain bandwidth. This indicates that IR scattering is the governing factor for the threshold current at low temperature [13]. The derived loss-bandwidth products are slightly smaller than those derived in [11] with another method. Further improvement of the threshold current density, the dynamic range, and the output power of the structures can be achieved by designing a structure with a longer effective lifetime. Minimizing the IR scattering time between the lasing states should be a promising approach to realize a high performance 3P-QCL [14].

| Device | $N_{3D}$ (cm$^{-3}$) | $J_{\text{th}}$(kA/cm$^2$) | $E_{\text{th}}$(kV/cm) | $T_{\text{max}}$(K) | $\nu$(THz) | $\tau_{\text{eff}}$(ps) | $f_{23}$ | $\tau_{\text{IR}}^{\text{th}}$(ps) | $\tau_{32}$(ps) |
|--------|-------------------|---------------------|-------------------|-------------------|----------|-------------------|--------|-----------------|--------------|
| V845   | $9 \times 10^{15}$ | 0.89                | 19.4             | 152              | 2.4      | 1.1               | 0.33   | 3.53            | 2.52         |
| V895   | $9 \times 10^{15}$ | 1.33                | 19               | 134              | 2.5      | 0.72              | 0.35   | 3.23            | 2.28         |
| V962   | $7.6 \times 10^{15}$ | 1.47                | 18.2             | 151              | 2.4      | 0.61              | 0.39   | 2.54            | 1.87         |
3. Intrasubband IR scattering in 3P-QCLs
In conventional RP structures, the gain bandwidth of the design is mainly determined by the tunneling coupling between either the injection state and the upper lasing state or that between the extraction state and the lower lasing state [15, 16]. In the 3P-QCLs, there is no state to be in resonance with either the upper or the lower lasing state, then the gain spectrum is not perturbed by tunneling effect. To compare how the pure dephasing time between the lasing states \( \tau^* = 2\hbar/\Gamma_{\text{intra}} \) changes from a RP-QCL to a 3P-QCL, we calculate the intrasubband IR scattering time between the lasing states in both RP and 3P-QCLs.

The intrasubband ion-impurity scattering time and the IR scattering time were calculated at designed electric field and different temperatures. Our calculation shows that the intrasubband ion-impurity scattering time of the RP-QCL presented in [2] is 0.75 ps at 50 K while the IR scattering time is 1.45 ps at 50 K. By using the dephasing time equation \( \tau^* = 2\hbar/\Gamma_{\text{intra}} \), the value of 1 ps is obtained which is comparable with the value reported in [2]. We calculated the intrasubband IR scattering time between the lasing states of the 3P-QCLs and the values of 0.16 ps, 0.24 ps, and 0.43 ps were obtained in V845, V962, and V895, respectively. The much shorter intrasubband IR scattering time between the lasing states in the 3P-QCLs is attributed to a higher energetic barrier and a lower oscillator strength compared to the RP-QCL presented in [2]. Our calculation shows that not only does IR scattering degrade the performance of the structure by lowering the effective lifetime and hence the population inversion of the structure, but it also may increase the gain bandwidth of the structure. However, these predictions on the effect of IR on gain bandwidth need to be confirmed experimentally, for instance by time-domain spectroscopy. Of course, impurity scattering is also at play in the bandwidth [18], therefore the position of doping should be carefully optimized [19].

4. Conclusion
The interface roughness scattering mechanism in THz QCLs based on 3P designs was investigated. The results indicate that the IR scattering might be the limiting factor on
the device performance, in particular for threshold current density at low temperature. Our modeling shows that not only can IR scattering increase the threshold current density of the structure by reducing the effective lifetime, but it also would increase the gain bandwidth of the design due to a shorter intrasubband IR scattering time between the lasing states. Any further improvement in THz 3P-QCLs may require precisely minimizing the IR scattering impacts on both effective lifetime and gain broadening of the quantum design.

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