Room-temperature, pulsed mode operation of a 9 µm GaAs/AlGaAs intersubband quantum cascade laser (QCL) has been accomplished1 by increasing the barrier-layer Al content from 33% to 45% within the conventional three-well active-region design. This important milestone in the mid-infrared (mid-IR) GaAs/AlGaAs QCL technology was achieved due to the larger conduction band offset in the 33%-Al device than the 33% one.2,3 With further increase of the barrier Al content, once the upper lasing level becomes aligned with the lowest X-valley state of the injection barrier, lasing is suppressed due to intervalley carrier transfer, which limits the emission wavelengths to above 8 µm.4 Moreover, satellite-valley leakage can play a significant role in the carrier loss in InP-based mid-IR QCLs.5 Therefore, it has become necessary to incorporate both Γ- and satellite-valley electronic transports into theoretical mid-IR QCL modeling. However, theoretical models6–11 published so far have focused on the Γ-valley transport alone.

In this letter, we present a three-dimensional (3D) Monte Carlo simulation of two GaAs-based mid-IR QCLs with equivalent designs (the 33%-Al QCL of Refs. 2 and 3 and the 45%-Al QCL of Ref. 1) that takes both Γ- and X-valley transports into account. Designs of these two QCLs are equivalent,1 since they have similar emitting wavelengths (~9 µm), threshold fields (48 kV/cm), dipole matrix elements (1.6 nm for the 33% QCL and 1.7 nm for the 45% QCL), and lifetimes in the upper lasing level (1.5 and 1.4 ps, respectively). Simulation reveals that the dominant X-valley leakage path in both lasers is X→X interstage scattering, exceeding the current due to direct interstage transfer between Γ and X valleys. The magnitude of the leakage current due to interstage X→X scattering depends on the occupation of the X-valley subbands, which are populated primarily by the same-stage scattering between the continuumlike Γ states (denoted as Γc for brevity) and the X-valley states. In the 33% QCL, localized Γ states (Γl for brevity) of the injector miniband couple strongly to the next-stage Γc states. Not only does this coupling lead to the well-recognized Γl→Γc leakage,2,12 but, through populating Γc, also indirectly ensures high X-valley occupation and subsequent high X→X leakage current at 300 K, even at low fields. Very good agreement with experiment is obtained at both cryogenic and room temperatures. © 2006 American Institute of Physics. [DOI: 10.1063/1.2387485]

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**X-valley leakage in GaAs/AlGaAs quantum cascade lasers**

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The authors present a Monte Carlo simulation of GaAs/Al0.33Ga0.67As and GaAs/Al0.45Ga0.55As quantum cascade lasers (QCLs) that incorporates both Γ- and X-valley transport. The dominant X-valley leakage path in both lasers is interstage X→X scattering. The leakage current is much higher in the 33%-Al QCL, as strong coupling of its weakly localized Γ-valley states to the next-stage continuum Γ states (Γc), followed by strong same-stage Γc→X scattering, ensures high X-valley population and subsequent high X→X leakage current at 300 K, even at low fields. Very good agreement with experiment is obtained at both cryogenic and room temperatures. © 2006 American Institute of Physics. [DOI: 10.1063/1.2387485]
growth direction, denoted as X1 states (mixing of the X1 and Γ subbands is neglected\(^{14}\)), and (ii) another set of doubly degenerate states, corresponding to the other two X valleys whose transverse axes are in the growth direction, denoted as X2 states.

Scattering mechanisms included are electron-LO-phonon and electron-electron (e-e) scattering among the Γ-valley subbands, X intravalley electron-LO scattering, and intervalley Γ-X and X-X scattering. Electron-phonon interaction is implemented assuming bulk phonons and quasi-two-dimensional electrons, while the e-e scattering is realized by employing the quasistatic multisubband screening model.\(^{15-27}\) For all the scattering mechanisms, we include both the intrastage and interstage scattering events, with the latter yielding the current flow through the whole QCL device. The current density \(J\) is defined in terms of the carrier flux exiting the simulated \(n\)th stage across its left and right boundaries.\(^ {10}\)

Figure 1 illustrates the electronic structure of the 33% QCL [Fig. 1(a)] and the 45% QCL [Fig. 1(b)] at 77 K and above-threshold field of 53 kV/cm. The number of X states in each stage is the same and chosen such that the highest X subband is right above the second Γ continuumlike state and below other higher X levels. Since the X band edge is about 83 meV above the Γ band edge in the 33% QCL but \(\sim\) 30 meV below the Γ band edge in the 45% QCL, more X subbands are needed to properly simulate the latter device. In particular, at \(F=53\) kV/cm and \(T=77\) K, nine (ten) X1 subbands and four (six) X2 subbands are used in the 33% (45%) QCL simulation.

In Fig. 2, the applied field versus current density characteristics are shown for the 33% QCL [Fig. 2(a)] and the 45% QCL [Fig. 2(b)], with and without the X-valley transport included. At the temperature of 77 K, the calculated threshold current \((J_{\text{th}})\) for the 33% QCL with the X-valley transport included is 4.4 kA/cm\(^2\) while the average experimental value is 5 kA/cm\(^2\) (see Fig. 3 of Ref. 3). For the 45% QCL, the calculated \(J_{\text{th}}\) is 2.9 kA/cm\(^2\) while the experimental value obtained in Ref. 1 equals 4 kA/cm\(^2\). Both threshold currents agree with the experimental data very well, especially considering that the simulation does not account for the losses at the lateral waveguide (ridge) edges. Subsequent experimental work\(^ {18}\) on 45% QCLs, where the ridge edges had smooth surfaces, due to wet chemical etching, and no absorbing material, reported \(J_{\text{th}}=3\) kA/cm\(^2\), in excellent agreement with our calculation. The 33% QCL shows higher \(J_{\text{th}}\) in both theory and experiment than the 45% QCL. At the low temperature of 77 K, this difference (about 1 kA/cm\(^2\) at threshold) is primarily due to strong \(\Gamma_{\text{c}}\)–Γ\(_{\text{c}}\) interstage leakage, stemming from poor localization of the Γ\(_{\text{c}}\) states in the 33% QCL and their large overlap with the next-stage Γ\(_{\text{c}}\) states [Fig. 1(a)]. X-valley transport in the 33% QCL amounts for a small additional leakage current (0.4 kA/cm\(^2\) at threshold). In the 45% QCL, the injector states are well localized and thus the leakage current due to both Γ\(_{\text{c}}\)–Γ\(_{\text{c}}\) interstage scattering and X-valley transport is negligible up to very high fields.

At room temperature, the simulated threshold current for the 33% structure with the X-valley transport included is 0.4 kA/cm\(^2\). In the 45% QCL, the injector states are well localized and thus the leakage current due to both Γ\(_{\text{c}}\)–Γ\(_{\text{c}}\) interstage scattering and X-valley transport is negligible up to very high fields.

FIG. 1. (Color online) Energy levels and wave function moduli squared in two adjacent stages for the 33% QCL (a) and the 45% QCL (b). In each stage, the bold black line denotes the upper lasing level, while the thin black lines and two bold green lines represent the localized Γ\(_{\text{c}}\) states and continuumlike Γ states, respectively. X1 states (red lines) and X2 states (blue lines) in two adjacent stages are also shown.

FIG. 2. Electric field vs current density characteristics for the 33% QCL (a) and the 45% QCL (b) at 77 and 300 K, with and without the X-valley transport included.
from the 33% QCL, owing to strong interstage carrier scattering. What is striking is how large the quantum efficiency is, comparing Figs. 2 and 3, at 300 K, the increase in the quantum efficiency does not account for ridge edge losses. As seen by the high fields, compared with the 33% QCL even at fields significantly below threshold. The simulated quantum efficiency is very good agreement with the 33% QCL could not lase at 300 K. For the 45% QCL, the quantum efficiency increases directly and is very efficient at room temperature in both lasers. The quantum efficiency is about 25.5 kA/cm². This is due to the fact that the X→X interstage scattering is the dominant leakage mechanism, more efficient than direct interstage scattering between X and X. What is striking is how large the X-valley leakage current is in the 33% QCL even at fields significantly below threshold. The increased X-valley leakage current even at low fields, in the 33% QCL at 300 K. In contrast, good localization of the injector miniband states in the 45% QCL ultimately leads to low X-valley leakage current up to high fields. The simulated Jth with the X-valley leakage included is in very good agreement with experiment for both QCLs at 77 and 300 K.

In summary, we have presented a Monte Carlo simulation incorporating the effects of X-valley transport on the operation of equivalent-design GaAs/Al0.33Ga0.67As and GaAs/Al0.44Ga0.55As QCLs. The 33% QCL has a higher X-valley leakage current than the 45% QCL at both 77 and 300 K. The reason is strong coupling between the injector states and the next-stage continuum-like states in the 33% QCL, which facilitates filling of the X-valley states through efficient intrastage scattering. With high X-valley occupation, intrastage X→X scattering yields a high leakage current, even at low fields, in the 33% QCL at 300 K.

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