Design and optimization of a GaAs-based sub-7-μm quantum cascade laser based on multivalley Monte Carlo simulation

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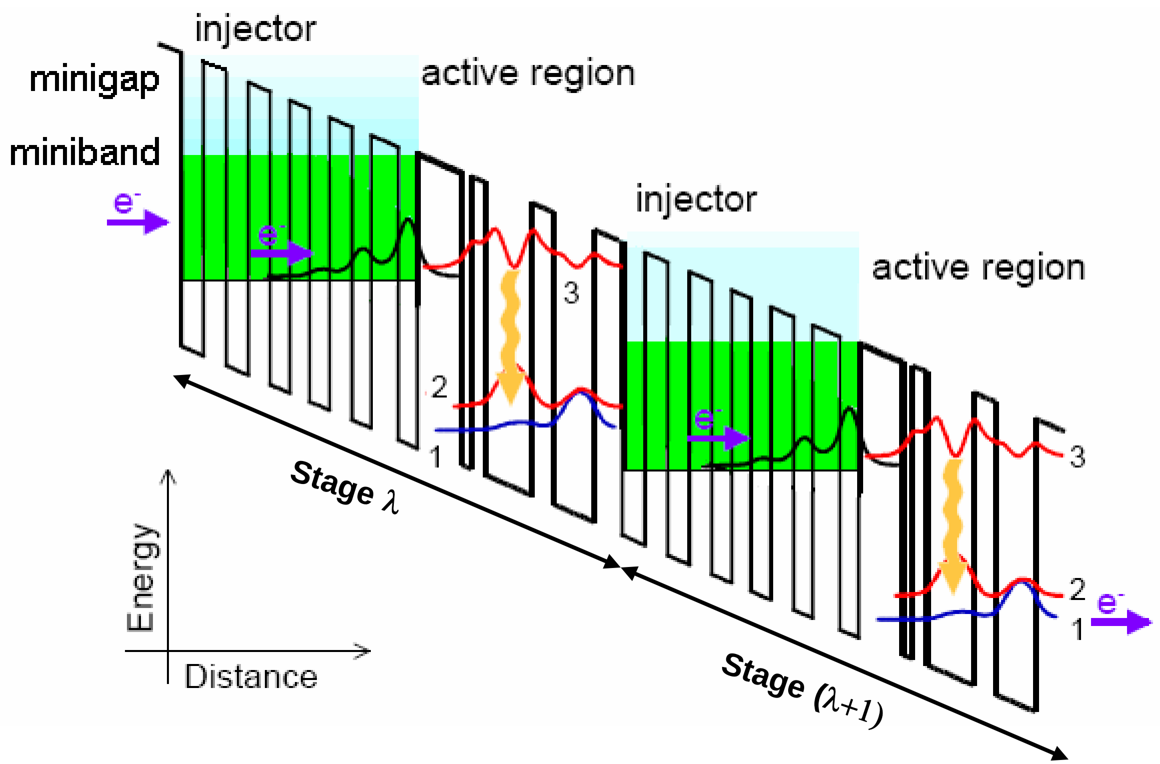
Quantum Cascade Lasers (QCLs) - Introduction



Principle:

- Quantum confinement
- Tunneling

Applications:

- Gas sensing
- Medical
- Telecomm.

Features:

- Unipolarity → Wide range of wavelengths: 3 to 160 μm
- Cascading scheme → One electron generates multiple photons

Motivation

Low wavelength limit in GaAs-based QCLs

Γ-X intervalley scattering

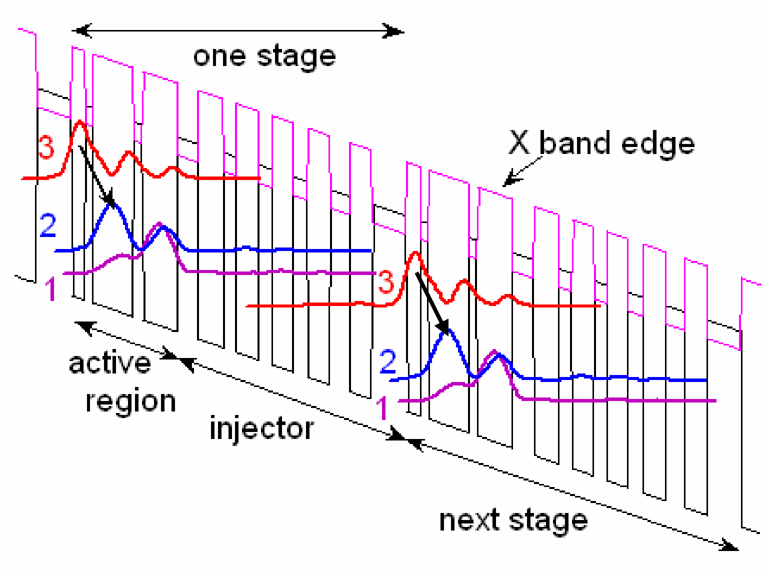
Wavelength of GaAs/AlGaAs QCLs $\geq$ 8 μm

Goal:

Design and optimize a novel GaAs QCL structure to emit below 7 μm with no penalty in device performance

Deep-active-well 6.7 μm GaAs QCL

State-of-the-art mid-IR GaAs QCL[1]



GaAs/$Al_{0.45}Ga_{0.55}As$

λ = 9.4 μm

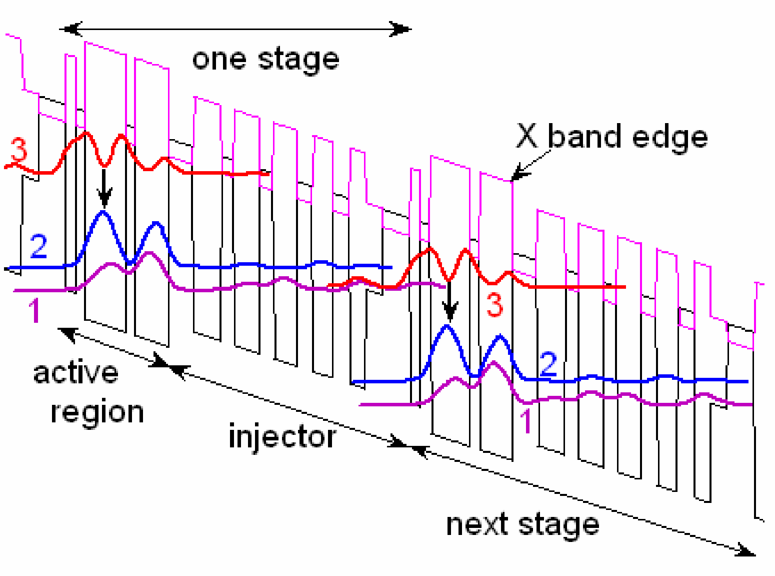
$\langle z_{32} \rangle$ = 1.7 nm

τ_3 = 1.4 ps

[1] H. Page *et al.*, APL **78**, 3529 (2001).

[2] X. Gao *et al.*, APL **89**, 191119 (2006).

Our deep-active-well structure



GaAs/$Al_{0.45}Ga_{0.55}As$

- Deep active wells: $In_{0.1}Ga_{0.9}As$

Barrier step: $GaAs_{0.6}P_{0.4}$

λ = 6.7 μm

$\langle z_{32} \rangle$ = 1.5 nm

τ_3 = 1.5 ps

Injector design by Multivalley

- **Monte Carlo simulator**

Transport Model in Mid-Infrared (IR) QCL Structures

Stationary charge transport in mid-IR QCLs described by the Boltzmann-like transport equation (BTE)[3-4]

$$\frac{d}{dt} f_{\mathbf{k}\alpha} = \sum_{\mathbf{k}'\alpha'} \left[S_{\mathbf{k}'\alpha',\mathbf{k}\alpha} f_{\mathbf{k}'\alpha'} \left(1 - f_{\mathbf{k}\alpha}\right) - S_{\mathbf{k}\alpha,\mathbf{k}'\alpha'} f_{\mathbf{k}\alpha} \left(1 - f_{\mathbf{k}'\alpha'}\right) \right]$$

$$S_{\mathbf{k}\alpha,\mathbf{k}'\alpha'} = \frac{2\pi}{\hbar} \left| \langle \mathbf{k}'\alpha' | H_{\mathrm{int}} | \mathbf{k}\alpha \rangle \right|^2 \delta(E_{\mathbf{k}'\alpha'} - E_{\mathbf{k}\alpha} \mp \hbar\omega)$$

Fermi's Golden Rule

$$|\mathbf{k}, \alpha\rangle = |\mathbf{k}, \nu\lambda\ell\rangle$$ ⟷ 3D single electronic state

In-plane wave vector

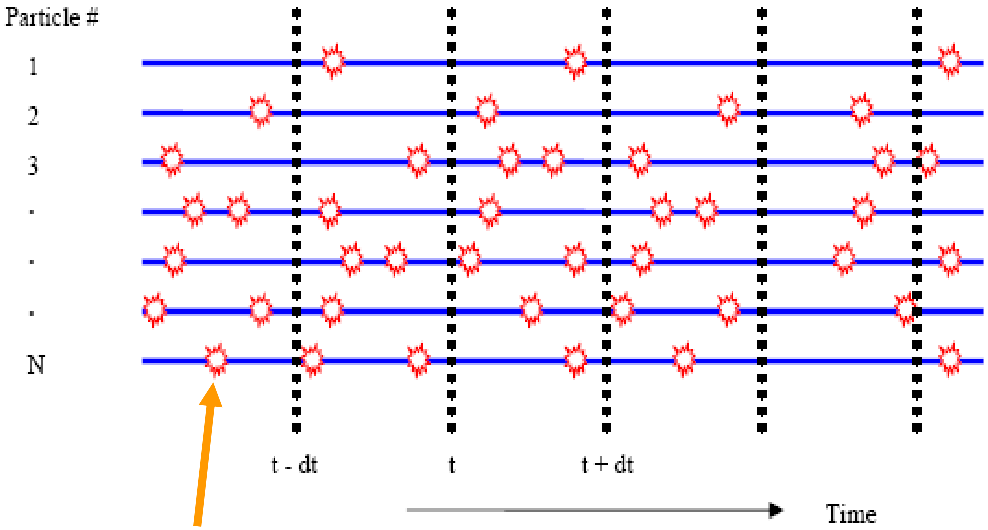
νth subband, λth stage, ℓth valley
(Γ, **X_z, X_x, and X_y valleys**)

[3] R. C. Iotti and F. Rossi, Phys. Rev. Lett. **87**, 146603 (2001).

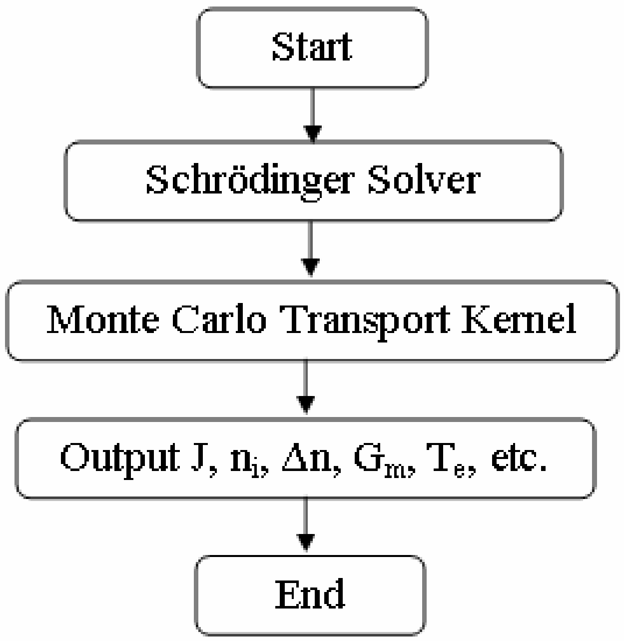
[4] X. Gao, D. Botez, and I. Knezevic, J. Appl. Phys. **101**, 063101 (2007).

Ensemble Monte Carlo (EMC) Method

EMC method - most accurate technique to solve BTE



Scattering event



Start

Schrödinger Solver

Monte Carlo Transport Kernel

Output J, n_i, Δn, G_m, T_e, etc.

End

- Random numbers determine the time between two consecutive scatt. events and the scatt. mechanism
- Distribution function **f** evaluated at each sampling time
- Macroscopic quantities (**J, n_i,** etc.) calculated from **f**

Electronic States

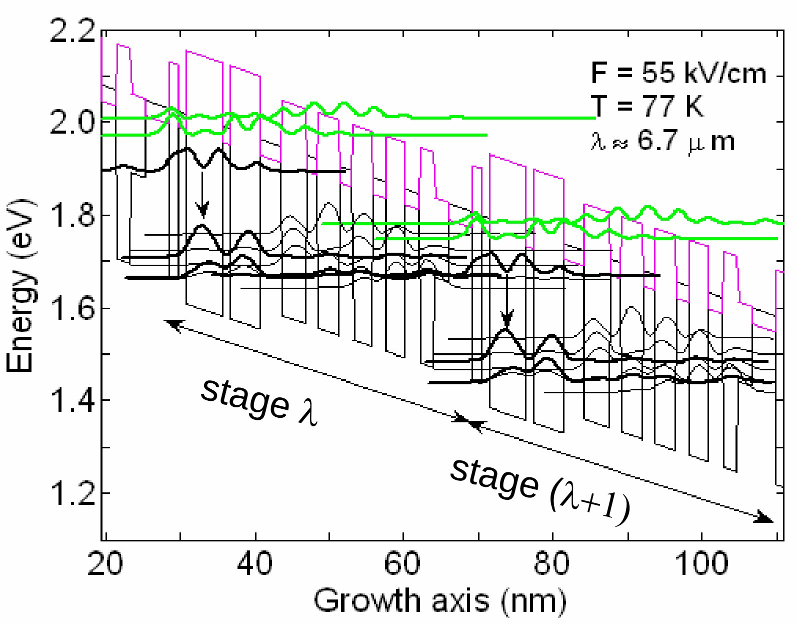
Electronic states in two adjacent stages

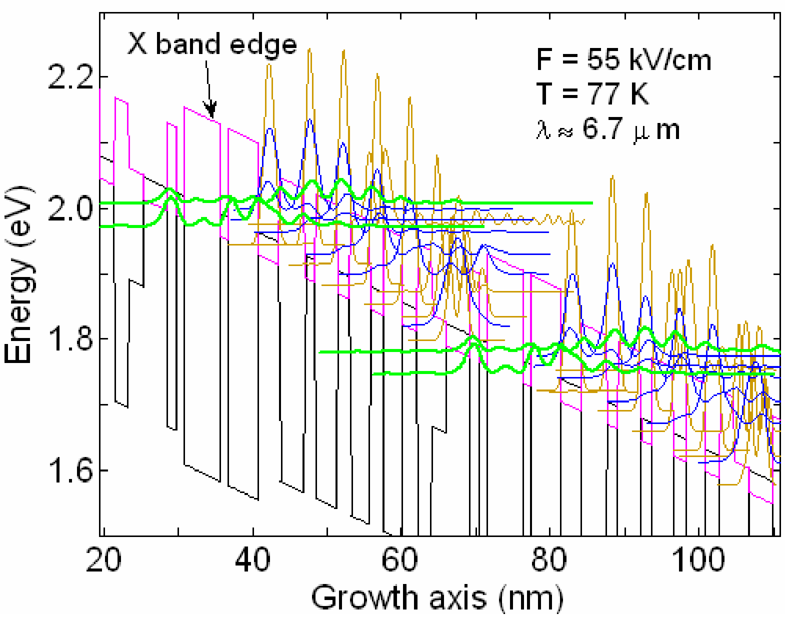
- Γ-states obtained using the **k . p** method
- X-states obtained using the effective mass equation

⇨ X_z, X_x, X_y valley states (X_x and X_y equivalent)

Γ-bound (black) and Γ-cont. (green) states

X_z (yellow) & X_x (blue) states





Scattering Mechanisms

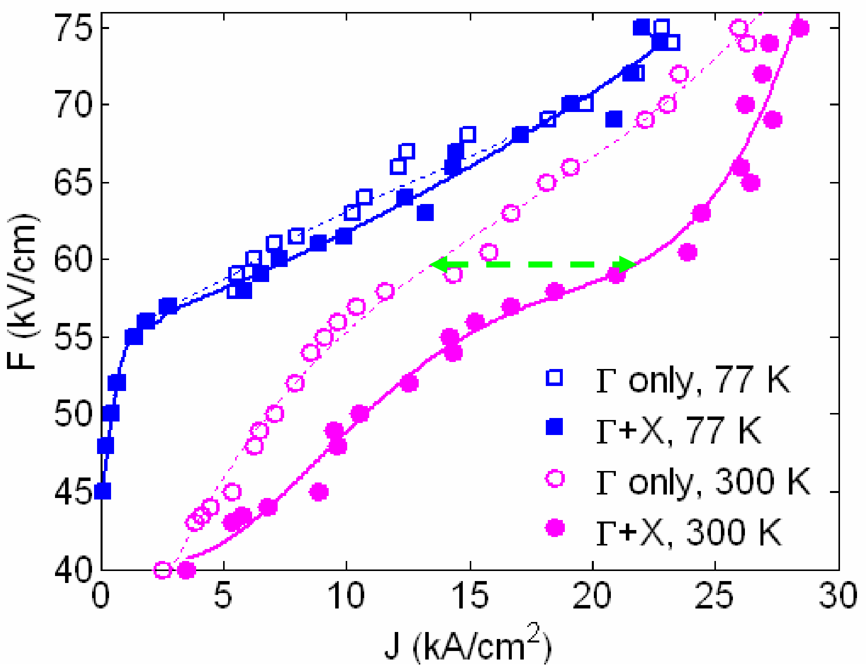
Scattering mechanisms included

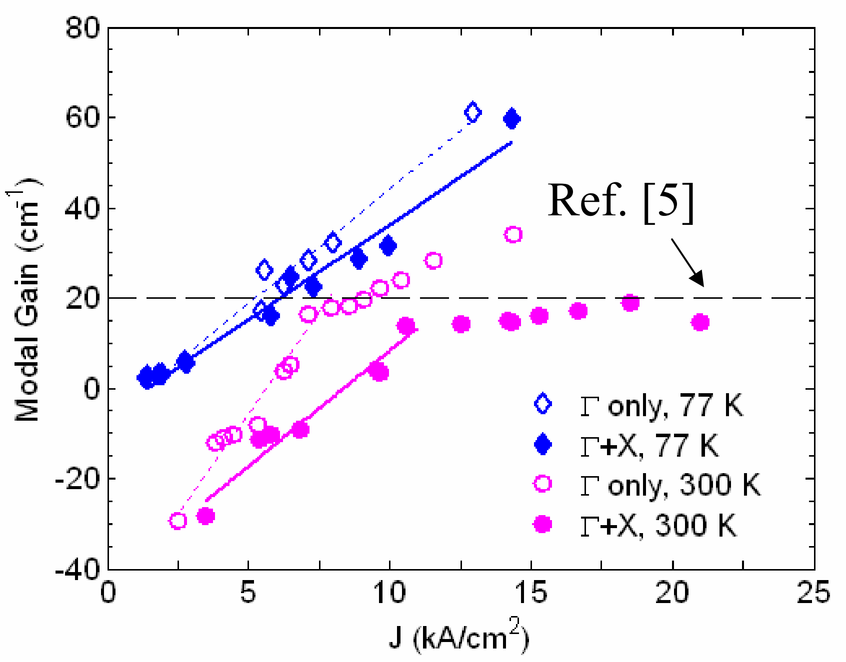
Intrastage $(\lambda \to \lambda)$ & Interstage $(\lambda \to \lambda \pm 1)$	**Γ-valley**	**X_z-valley**	**X_x-valley**
	Electron-LO Electron-Electron $\Gamma \to X_z$ $\Gamma \to X_x$	Electron-LO $X_z \to \Gamma$ $X_z \to X_x$	Electron-LO $X_x \to \Gamma$ $X_x \to X_z$ $X_x \to X_x$ (*)

- ➢ Interstage scattering gives rise to the current
- ➢ LO and intervalley phonons treated as bulk phonons

(*) Due to the double-degeneracy of X_x-valley

Simulation of Initial Structure A



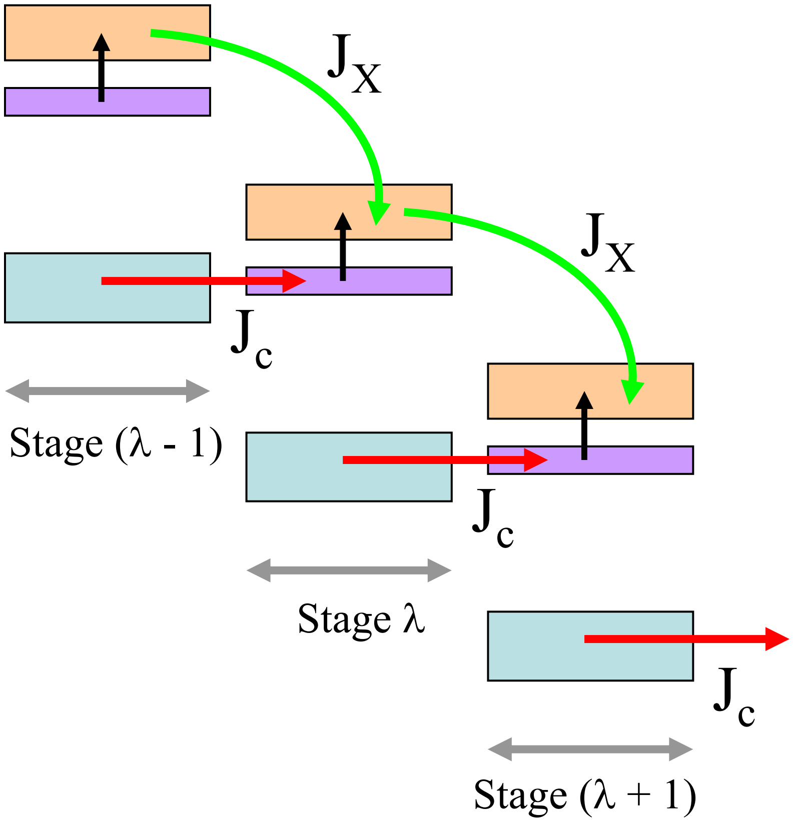


Issues with structure A

- Large X-valley leakage current at room temperature (RT)
- Insufficient modal gain for RT operation

[5] X. Gao, M. D’Souza, D. Botez, and I. Knezevic, J. Appl. Phys. *submitted* (2007).

Dominant X-valley Leakage Mechanism[4]



🟦 Injector states

🟪 Γ-continuum states

🟧 X-states

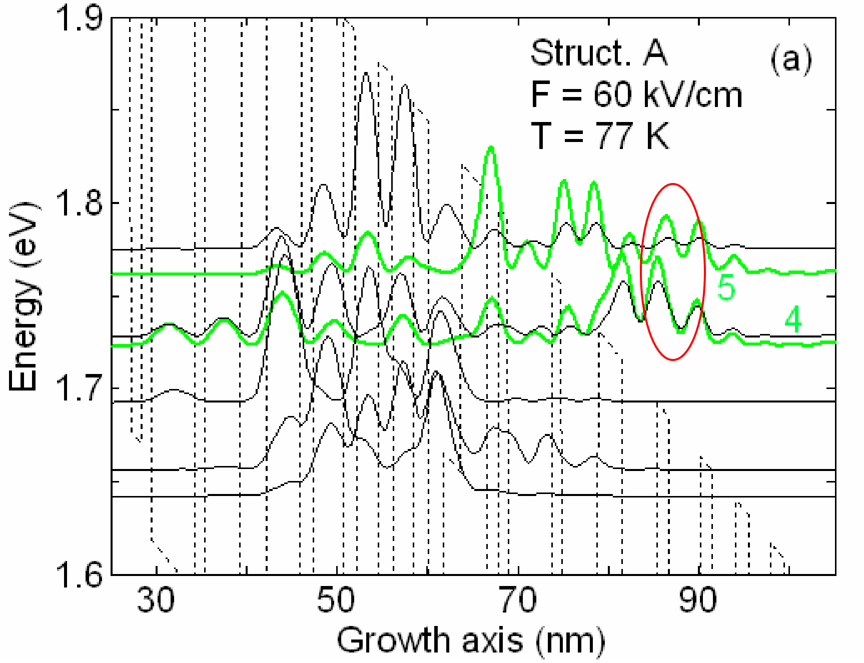
Dominant X-valley leakage current path: J_X

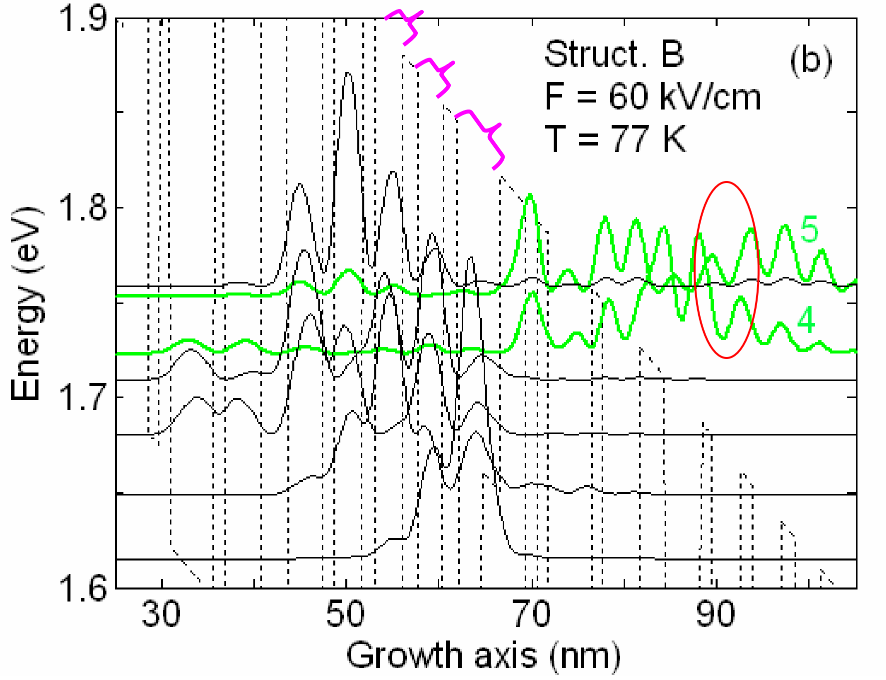
Minimize the overlap between injector and Γ-continuum states

→ $J_c \downarrow$, $J_X \downarrow$

[4] X. Gao, D. Botez, and I. Knezevic, J. Appl. Phys. **101**, 063101 (2007).

Injector-Γ_c Wavefunction Overlap





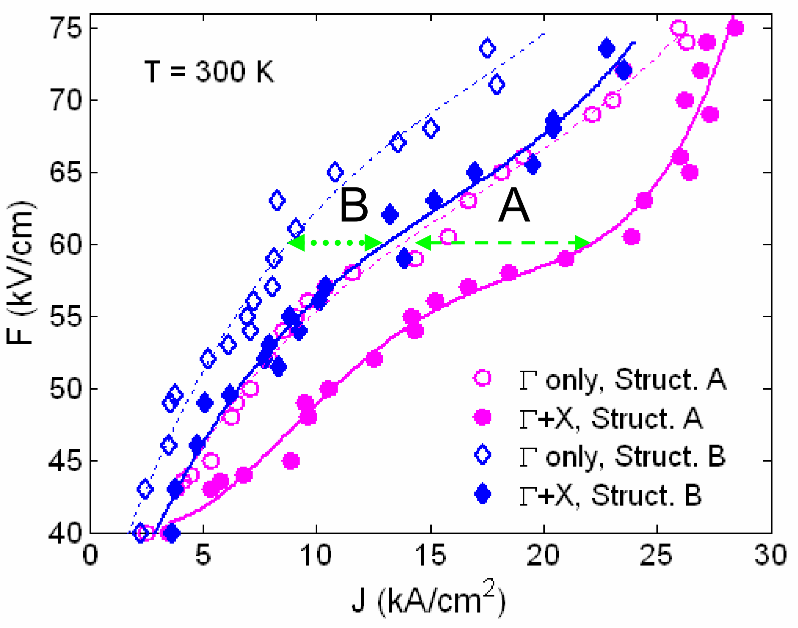
Strong coupling between injector Γ-bound states (thin black) and Γ_c-states (green)

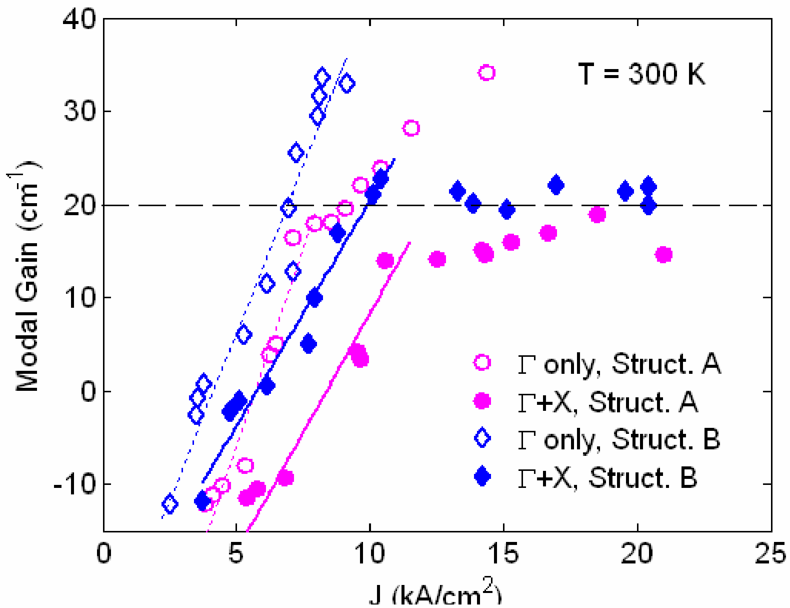
- Large X-valley leakage current at RT
- Insufficient modal gain for RT operation

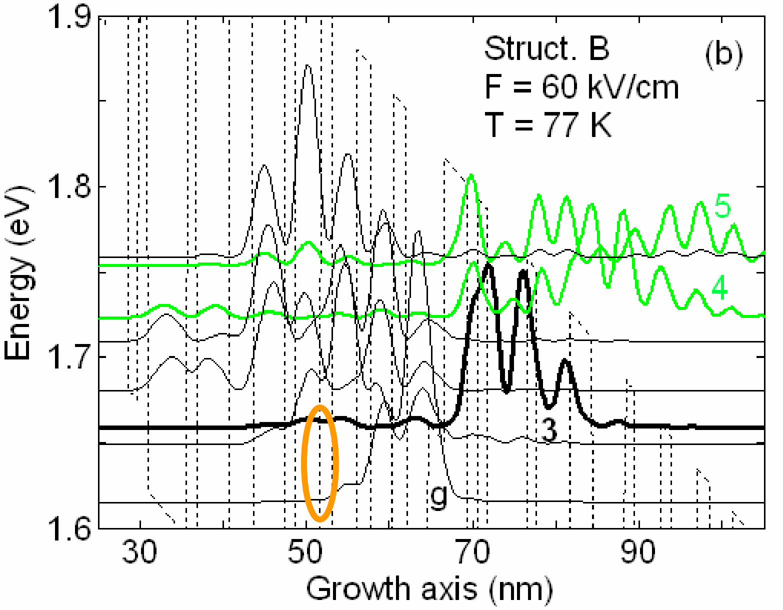
Increased injector well thickness

- **Reduced coupling between injector and Γ_c-states**

Improved Structure B



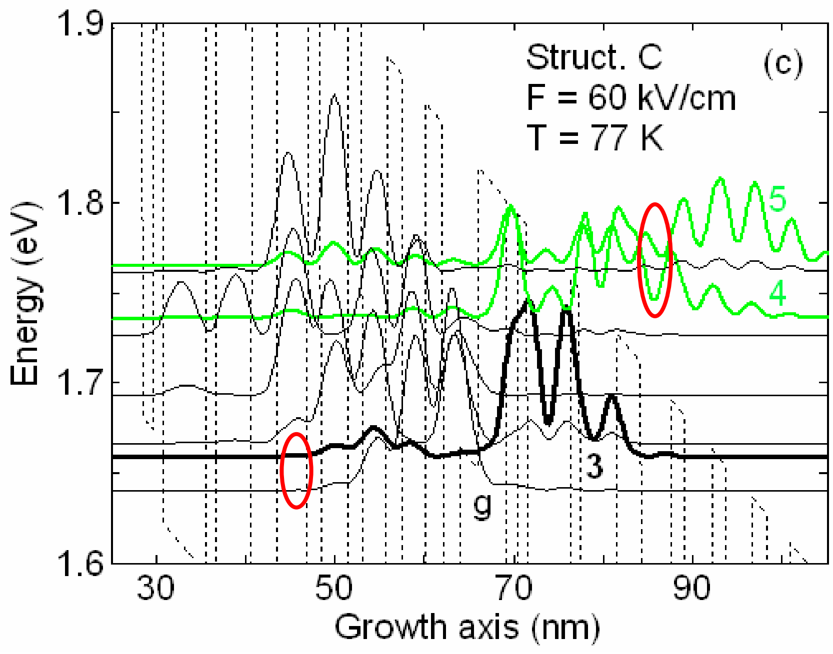


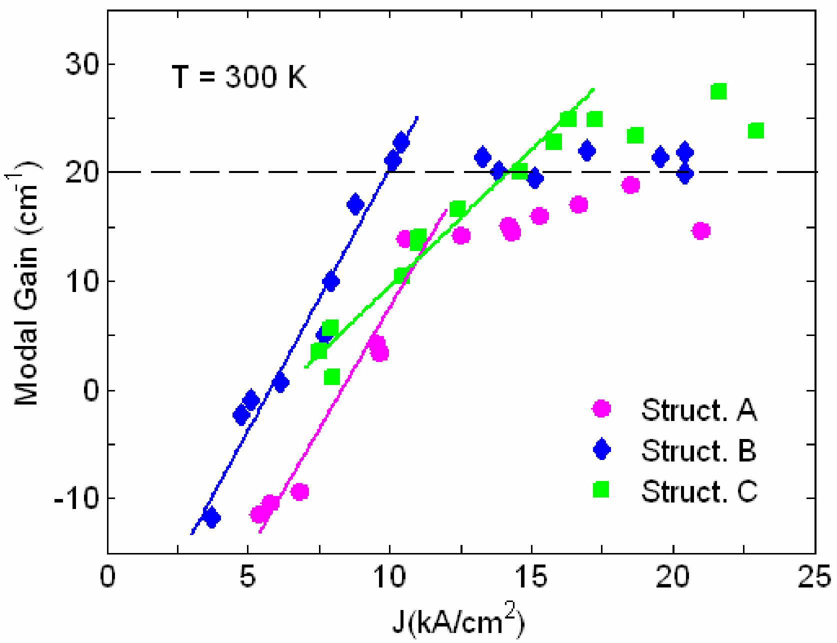


- Reduced X-leakage
- Saturation gain = loss at 300 K
- Gain < loss at 77 K

Large separation between level 3 and injector ground level g

Optimized Structure C





- Reduced coupling between injector and Γ_c-states
- Decreased energy difference between levels 3 and g

	77 K	300 K	300 K
	J_{th} (kA/cm^2)	J_{th}	T_e (K) @ J_{th}
6.7 μm (Struct. C)	**5**	**14**	**530**
9.4 μm - Theory [2]	3	14.4	544
9.4 μm - Exper. [1]	4	16.7	

[1] H. Page *et al*., APL **78**, 3529 (2001).
[2] X. Gao *et al*., APL **89**, 191119 (2006).

Conclusion

- Proposed a deep-active-well design that enables shorter wavelength emission in GaAs-based QCLs.
- Optimized the injector layer thickness for desired device performance by using the Multivalley Monte Carlo (MMC) simulator developed.
- Optimized deep-active-well GaAs QCL allows to shorten the emission wavelength from 9.4 μm to 6.7 μm with no penalty in device performance.
- The deep-active-well design for shortening wavelength is extendable to InP-based QCLs, and the MMC simulator can be used for optimization of a wide variety of QCLs.