The Effects of Temperature on the Gain Profile of THz Quantum Cascade Lasers

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Motivation and Outline

What is limiting high temperature operation of THz QCLs?

Theoretical investigation of a THz QCL.

- Discuss the method.
- Present results.
- Try to interpret results.

What can be done to increase the temperature range?

Non-Equilibrium Green's Functions

- Main advantage: BROADENING. Extension of the density matrix:

$$\rho_{\alpha\beta}(\mathbf{k}) = -\mathrm{i} \int \frac{\mathrm{d}E}{2\pi} G^{<}_{\alpha\beta}(\mathbf{k}, E)$$

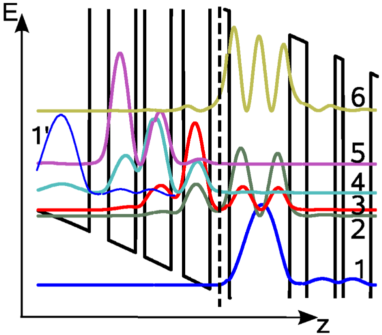
- Scattering due to Impurities, Interface roughness, Optical and Acoustic phonons, and also electron-electron interaction.
- No fitting parameters are used, only well-known material parameters.

The Calculation Procedure

1. Calculate the eigenstates states of the periodic laser structure.
2. Iterate to self-consistency:
   - Evaluate the Self-energies from the Greens functions.
   - Evaluate new Green's Function using the Dyson Equation and the Keldysh Relation.
3. The gain is calculated from the steady-state solution to the transport problem.

Conduction Band Profile

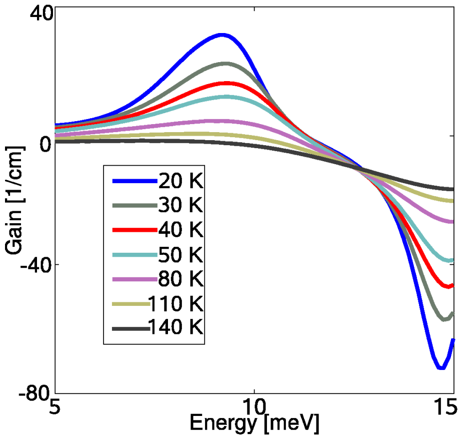
Resonant phonon depopulation design from the MIT group.



- Doping density $N_D = 2.25\text{x}10^{10}$ cm^{-2}.
- Emitting at 1.9 THz (7.9 meV).
- Lasing transition between state 4 and 3.
- Laser operation up to 110 K pulsed, 95 K cw.

Presented in S. Kumar *et. al.* APL **88**, 121123 (2006).

Gain



Strong decrease of peak gain with increasing temperature.

Increased broadening of both gain and absorption peak.

Bias 46.5 mV/period.

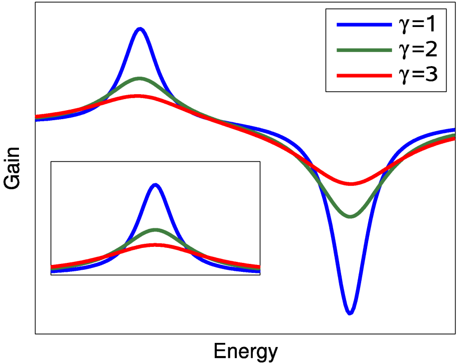
Broadening and Overlap - Simple Model

Lorentzian peaks:

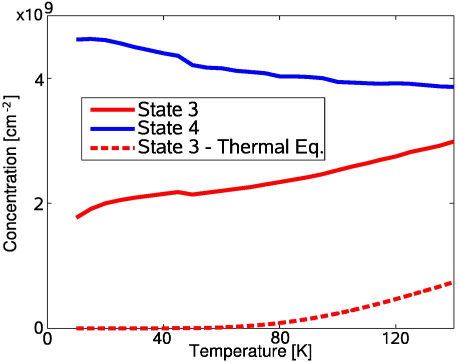
$$g(E) = \frac{1}{\pi} \frac{\gamma}{E^2 + \gamma^2}$$

where γ is the width.

Reduction *both* due to broadening and overlap.



Population inversion

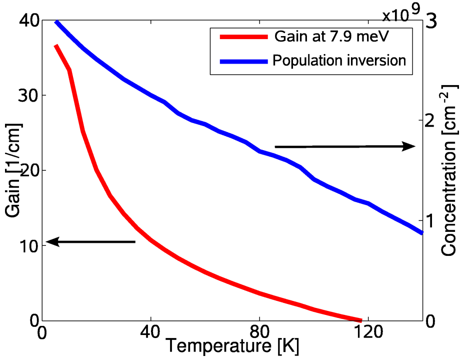


50 % reduction in inversion from low temperature to 100 K.

The increased population in the lower laser state is due to thermal backfilling.

Population inversion (2)

Gain at the lasing energy and the population inversion.



Maximum lasing temperature is in good agreement with experiment (110 K).

Population inversion but no gain.

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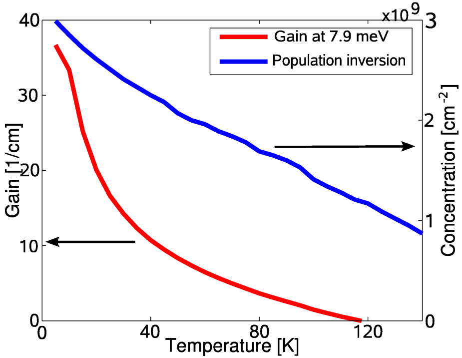

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Why?

Temperature Dependent Effects

Temperature enters our calculation in three ways:

- *Optical phonon scattering*. Emission is proportional to $n_B(\hbar\omega_{\mathrm{opt}}) + 1$. At T = 100 K, $n_B(\hbar\omega_{\mathrm{opt}}) \sim 10^{-2}$ in GaAs.
- *Acoustic phonon scattering*. Very weak coupling.
- *Impurity scattering*. Strongly influenced by the screening of ionised dopants by electrons. A common approach is the Debye-approximation,

$$V_{\mathrm{eff}}(r) = V_{\mathrm{coul}}(r)\mathrm{e}^{-\lambda_{\mathrm{Debye}} r}$$

and where the screening length is temperature dependent,

$$\lambda^2_{\mathrm{Debye}} = \frac{e^2 n_{\mathrm{3D}}}{\epsilon_s \epsilon_0 k_B T}.$$

A hot electron gas is less affected by the impurity potential $\Longrightarrow$ Less screening and more scattering.

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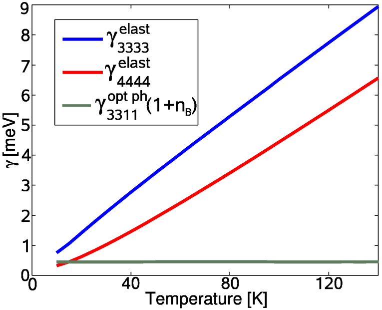
The γ-factors

Used when calculating the self energies

$$\Sigma_{\alpha\alpha'}(\mathbf{k}, E) = \sum_{\beta\beta'} \sum_{\mathbf{k}'} \gamma^{\text{elast}}_{\alpha\alpha'\beta\beta'}(\mathbf{k} - \mathbf{k}') G_{\beta\beta'}(\mathbf{k}', E)$$

where the rate $W_{\alpha\to\beta} = \frac{2\pi}{\hbar}\gamma_{\alpha\alpha\beta\beta}$



- Strong increase in the impurity scattering.
- Optical phonon emission is almost constant.
- $\gamma^{\text{ac}}_{3333} = 3.8\ \mu\text{eV}$ at 100 K.

Outlook

Can one reduce scattering from ionised dopants?

- Increase the energy of state 5 to reduce spectral overlap with the gain transition.
- The Debye screening length $l_{\mathrm{Debye}} = 1/\lambda_{\mathrm{Debye}} = 39$ nm at 100 K, the laser period length is 55.4 nm.
- Higher doping?

$$\Delta n \propto N_D \qquad \gamma \propto N_D \qquad l_{\mathrm{Debye}} \propto \sqrt{T/N_D}$$

Outlook - Simulation

- Screening of impurities is a complex many-body problem.
- Screening in electron-electron scattering should be just as important.

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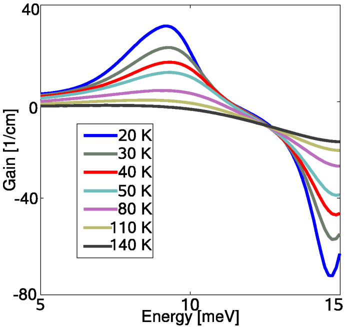
Conclusion

The NEGF simulation of a THz QCL has shown that:

- A substantial population inversion remains at maximum lasing temperature.
- Increased broadening of both gain and absorption transition reduce the gain peak height.
- The reason might be increased scattering from ionised dopants.



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