Influence of electron-phonon scattering in quantum dot cascade lasers

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Introduction

Quantum dots (QDs) are promising candidates as the semi-conductor gain medium for THz QCLs to reach room temperature operation. However, there has not been many models that are both intuitive and detailed enough to realistically simulate its operation characteristics. Model approaches include non-equilibrium Green's functions [1], which can be overly complex, and polaron density matrix [2], which can be difficult to use if many states and transitions are involved. Here we present results from a time-local density matrix model within the second-order Born-Markov approximation, accounting for coupling to both LA and LO phonons to calculate for the operation characteristics of a THz QDCL.

Comparison of Different Model Approaches

Model	Pros	Cons
NEGF [1]	Valid for all interaction strengths	Numerical complexity
Interaction approach (our work)	Easy to enumerize	Not valid for strong coupling, however still experimentally relevant
Polaron DM [2]	Valid for strong coupling	Difficult to enumerize for many transitions

Figure 1: Comparison of the available model approaches in the literature.

Structure Under Study

The quantum design under study at an electric field of 16 kV/cm is shown in Figure 2. Starting from the injector barrier, the design layer thicknesses are 3.7/8.2/3.8/16.8 nm GaAs/$Al_{0.2}Ga_{0.8}As$. Cylindrical basis is assumed – the wavefunctions are $\Psi(z,r,\theta) = \frac{1}{\sqrt{2\pi}}\psi(z)R(r)e^{im\theta}$

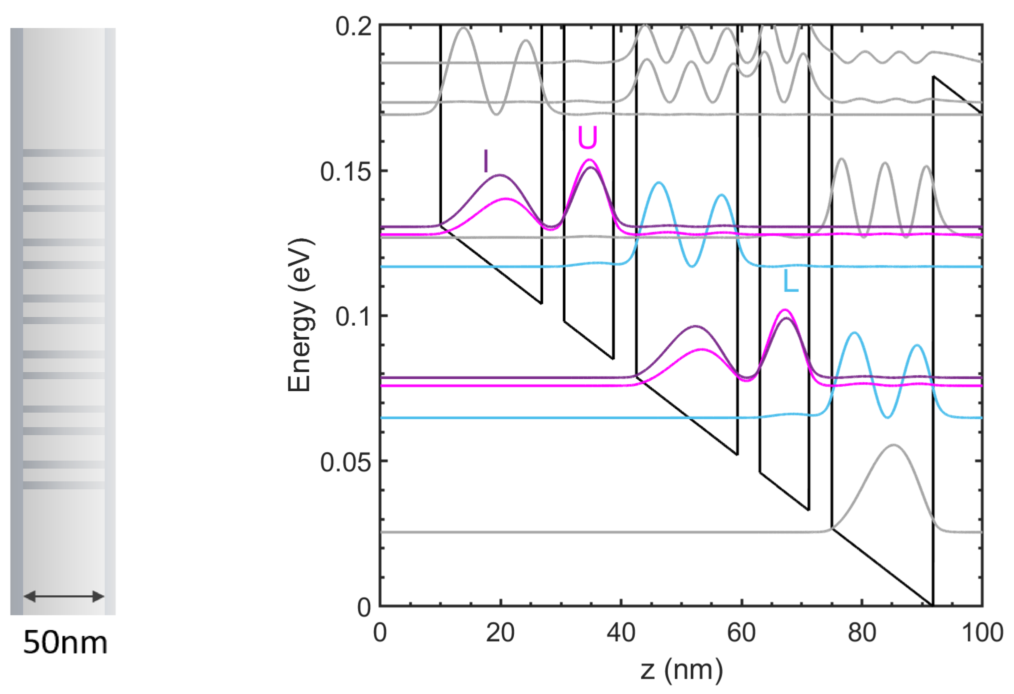

Figure 2: Schematic of the nanowire (left) and the band structure diagram (right) – colored lines indicate the states (wave functions) included in the simulation

Model

Transport

- LA and LO phonons are taken into account using a time-local master equation approach under the Markov approximation
- A generalized scattering formulation with a delocalized basis was then used, in order to be basis-invariant in accounting for the scattering processes [3].
- The system Hamiltonian is:

$$H = H_0 + H_{\rm opt} + H_{\rm e-ph}$$
$$= \sum_i E_i |i\rangle\langle i| + \sum_{nm} \Omega^{\rm opt}_{nm}(t)(|n\rangle\langle m| + |m\rangle\langle n|)$$
$$\sum_{nm}\sum_q V^{\rm LO}_q |n\rangle\langle m| (b_q + b^\dagger_{-q}) + \sum_{nm}\sum_q V^{\rm LA}_q |n\rangle\langle m| (b_q + b^\dagger_{-q}) \quad (1)$$

- which yields the main density matrix equation

$$\frac{d\rho}{dt} = \frac{1}{i\hbar}[H_0 + H_{\rm opt}, \rho] + \sum_{CD} \Gamma_{AB,CD}\rho_{CD} \quad (2)$$

where the scattering superoperator taking into account the e-phonon interactions is

Scattering Superoperator

$$\Gamma_{\substack{AB,CD\\0;\ 0}} = \sum_\sigma \sum_\pm \left(N_q + \frac{1}{2} \pm \frac{1}{2}\right)\Bigg[V_{\substack{AC,DB\\0,\sigma;\ \sigma,0}} \frac{e^{i(\omega_{CA+\sigma U} \mp \omega_q)t}e^{-\gamma t} - 1}{i(\omega_{CA+\sigma U} \mp \omega_q) - \gamma}$$
$$+ V_{\substack{AC,DB\\\sigma,0;\ 0,\sigma}} \frac{e^{i(\omega_{BD+\sigma U} \pm \omega_q)t}e^{-\gamma t} - 1}{i(\omega_{BD+\sigma U} \pm \omega_q) - \gamma}$$
$$- \delta_{B,D}\sum_F V_{\substack{AF,FC\\\sigma,0;\ 0,\sigma}} \frac{e^{i(\omega_{CF+\sigma U} \mp \omega_q)t}e^{-\gamma t} - 1}{i(\omega_{CF+\sigma U} \mp \omega_q) - \gamma}$$
$$- \delta_{A,C}\sum_F V_{\substack{DF,FB\\0,\sigma;\ \sigma,0}} \frac{e^{i(\omega_{FD+\sigma U} \pm \omega_q)t}e^{-\gamma t} - 1}{i(\omega_{FD+\sigma U} \pm \omega_q) - \gamma}\Bigg] \quad (3)$$

here σ is the sum over modules, U is the energy drop over different modules, A,B,C,D,F denote the indexing of the electronic eigen states, γ is the decay rate of the phonon (finite LO phonon lifetime was included), ω_q is the frequency of the phonon, and N_q is the Bose Eistein distribution.

Gain

- The optical field is included through

$$H_{\rm opt} = e\hat{z}E_{\rm ac}\cos(\omega t) \quad (4)$$

- The gain was calculated through the linear polarization / susceptibility [2] for the non-lasing conditions. When including the optical field, an evolution in time was implemented. The gain is given by

$$G(\omega) = \frac{\omega N_{3D}}{n_r c \epsilon_0}{\rm Im}\left(\frac{P(\omega)}{|E(\omega)|}\right) \quad (5)$$

Results

- Comparison of the gain spectra with/without LA phonons in Figure 3 shows that LA phonons help to achieve a higher population inversion for the main lasing transition (U to L) at low temperatures. We find a non-negligible energy shift for the lasing transitions due to the e-phonon interactions.

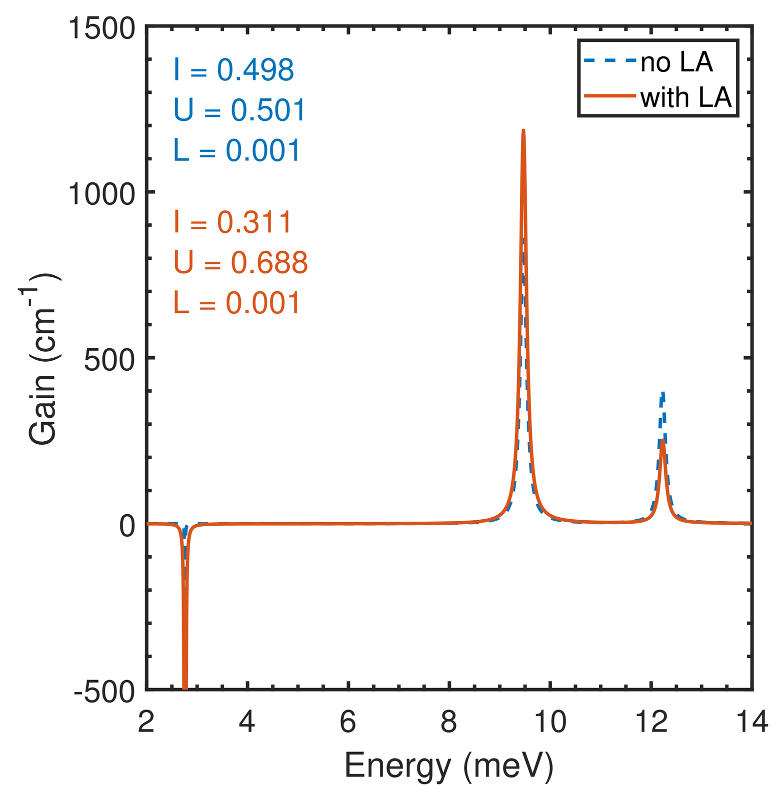

Figure 3: Gain calculated at T = 0K, with (orange solid) and without (blue dashed) LA phonons. Only s states ($m = 0$) were included.

- Figures 4 and 5 shows the gain calculated at 50 K and 300 K when including more states. Due to the long computation time, only selected LA phonon interactions were included. Multiple peaks appear due to those states having different energy shifts from the e-phonon interactions.

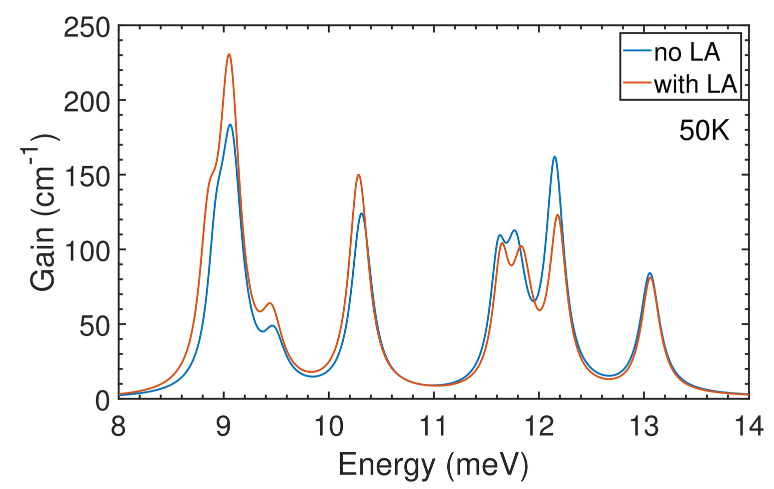

Figure 4: Gain calculated at 50 K, with and without LA phonons.

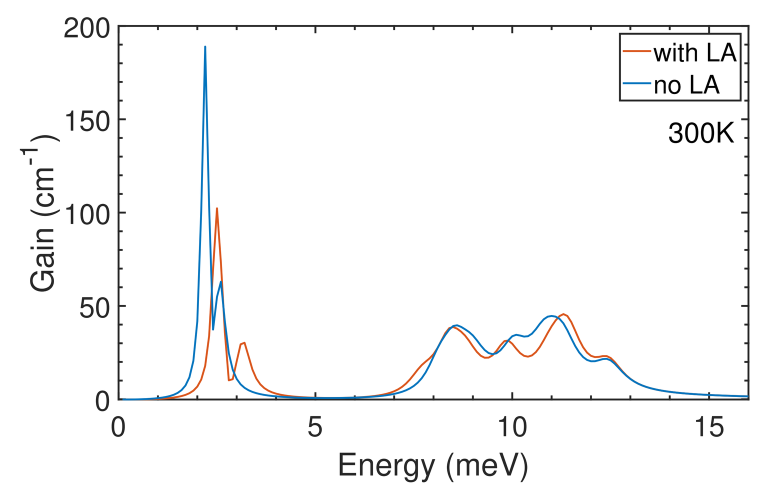

Figure 5: Gain calculated at 300 K, with and without LA phonons.

- Figure 6 shows a decrease of the gain as the lasing field strength is increased

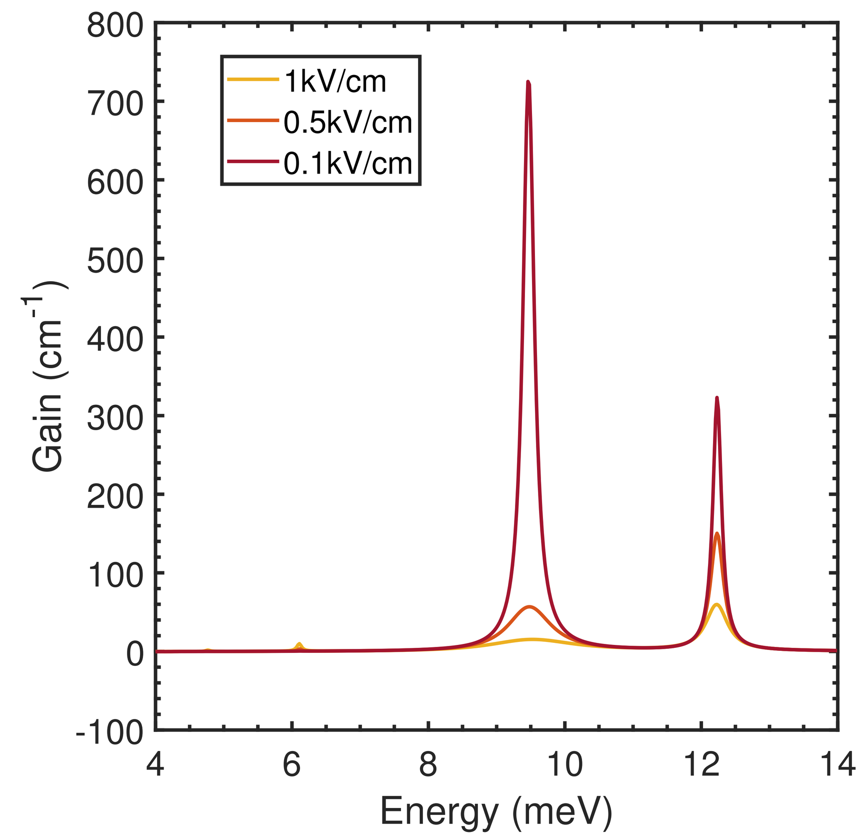

Figure 6: Gain spectra at T=0 K as a function of the lasing field strength.

Conclusions

- We have developed an intuitive and accurate master equation model to calculate for the operation characteristics of QDCLs
- This model is valid for weak to intermediate e-phonon interaction strength
- Our model shows that LA phonons can help to achieve a higher population inversion at low temperatures, and this should be considered in future QDCL designs
- Future work could include the addition of other scattering mechanisms such as interface roughness, ionized impurities, and possibly e-e- scattering – as well as code optimizations

References

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