IX International School and Conference on Photonics
August 28 - September 01, 2023, Belgrade

Dependence of Transport Parameters on Interface Composition Diffusion and Doping Segregation in Longitudinal Optical Phonon, Bound to Continuum and Hybrid THz Quantum Cascade Laser Designs

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1. Introduction

Quantum cascade lasers (QCLs) are semiconductor lasers with emission frequencies ranging from the mid-IR to the THz part of the spectrum, that can be designed by varying layer thicknesses and composition [1]. Due to the unique THz light emission of QCLs many designs have been developed, the most important of which are the Longitudinal Optical Phonon (LO), Bound to Continuum (BTC) and Hybrid designs [2]. These devices are grown at high temperatures by molecular beam epitaxy which makes them prone to diffusion of added barrier material that leads to interface composition diffusion which can have a prominent effect of QCL operation [3]. Doping segregation, that is the diffusion of the charged dopants, which changes the doping profile and effects the Hartree term in the total effective potential energy is also present in real QCLs.

2. Theoretical model

In this work both interface diffusion and doping segregation was modelled by numerically solving Fick's law with the finite difference method for the composition x and doping profile N_d. In the case of 1D structures Fick's law can be written and discretized as:

$$\frac{\partial x(z,t)}{\partial t}=D_x\frac{\partial^2 x(z,t)}{\partial z^2}\longrightarrow\frac{x(z_i,t_{j+1})-x(z_i,t_j)}{dt}=D_x\frac{x(z_{i+1},t_j)-2x(z_i,t_j)+x(z_{i-1},t_j)}{dz^2}$$

$$\frac{\partial N_d(z,t)}{\partial t}=D_N\frac{\partial^2 N_d(z,t)}{\partial z^2}\longrightarrow\frac{N_d(z_i,t_{j+1})-N_d(z_i,t_j)}{dt}=D_N\frac{N_d(z_{i+1},t_j)-2N_d(z_i,t_j)+N_d(z_{i-1},t_j)}{dz^2}$$

where dz and dt are incremental values od the coordinate and time grid respectfully. For each value of time the composition and doping profile are calculated for the entire structure using the values in the previous time value. This is repeated for a certain diffusion time t that is related to the diffusion length $L_d=\sqrt{Dt}$.

By diffusing the composition, we have not only described a more realistic conduction band offset $U_c(z)$, but also the effective mass along the growth direction $m^*(z)$ which are functions of the alloy composition x. Diffusion of the doping profile changes the Hartree term $(-e\varphi)$ in the total effective potential energy $U_{eff}(z)$ in the 1D effective mass Schrödinger equation which describes the electron structure of the QCL:

$$-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m^*(z)}\frac{d\psi_i(z)}{dz}+U_{eff}(z)\psi_i(z)=E_i\psi_i(z)\qquad U_{eff}(z)=U_c(z)-eKz-e\varphi(z)$$

where $\psi_i(z)$ is the envelope function, E_i is the electron energy and K the electric field.

In this contribution we investigate the dependence of transport parameters such as material gain, current density and emission frequency in the negative differential resistance (NDR) point on interface composition diffusion and doping segregation in the three most common THz QCL designs. The NDR point defines the maximum current density at which the QCL can operate, while operation starts at material gain equal to the threshold value. The transport of these devices was modelled by the density matrix model which takes into account quantum coherence effects and so adequately describes resonant tunneling through the injection barrier [4].

The density matrix model is a quantum mechanical model that takes into account coherence effects and uses the eigenstate basis of one QCL period for creating a statistical ansamble of all possible interactions in the system. The time evolution of the density matrix operator is given by the Liouville equation where the relaxation term describes dephasing scattering caused by elastic intrasubband scattering such as interface roughness and electron-impurity scattering that are not in the Hamiltonian.

$$\hat{\rho}=|\hat{\psi}(t)\rangle\langle\hat{\psi}(t)|\qquad\frac{d\rho}{dt}=-\frac{i}{\hbar}[H,\rho]-\left(\frac{d\rho}{dt}\right)_{relax}$$

The most important QCL transport characteristics are current density and material gain. In this model the current density j is found as the expected value of the drift current J, where n_{2D} is the electron sheet density, L_p the QCL period length and Z_s the dipole matrix:

$$j=Tr(\rho J)\qquad J=\frac{ien_{2D}}{\hbar L_p}[H,Z_s]$$

For an external EM field $A=A_0e^{i\omega t}+A_0e^{-i\omega t}$ the Hamiltonian and density matrix operator can be written:

$$H=H^{dc}+H^{ac+}e^{i\omega t}+H^{ac-}e^{-i\omega t}\qquad\rho=\rho^{dc}+\rho^{ac+}e^{i\omega t}+\rho^{ac-}e^{-i\omega t}$$

While the polarization of a isotropical linear medium is equal to $P=\varepsilon_0\chi_{opt}A$ where χ_{opt} is the optical susceptibility whose imaginary part can be found:

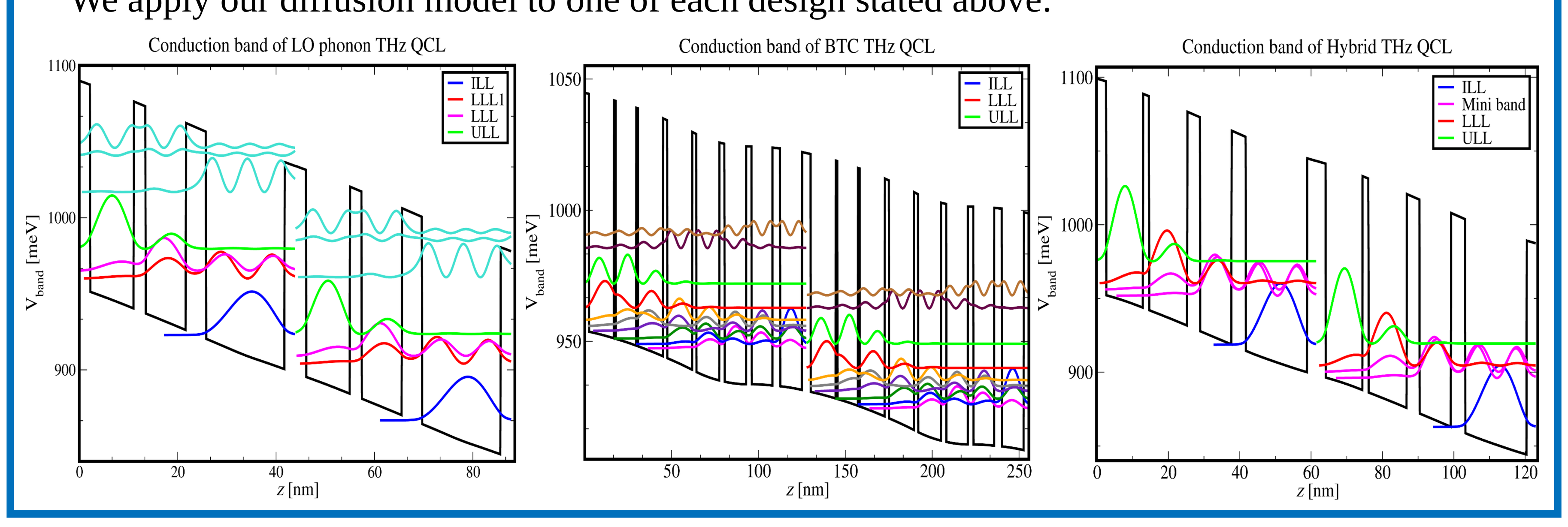
$$\mathrm{Im}\{\chi_{opt}\}=\frac{en_{2D}}{\varepsilon_0A_0L_p}Tr\left(\rho^{ac+}Z\right)$$

where Z is a part of the dipole matrix Z_s that corresponds to one QCL period.
The material gain is found as:

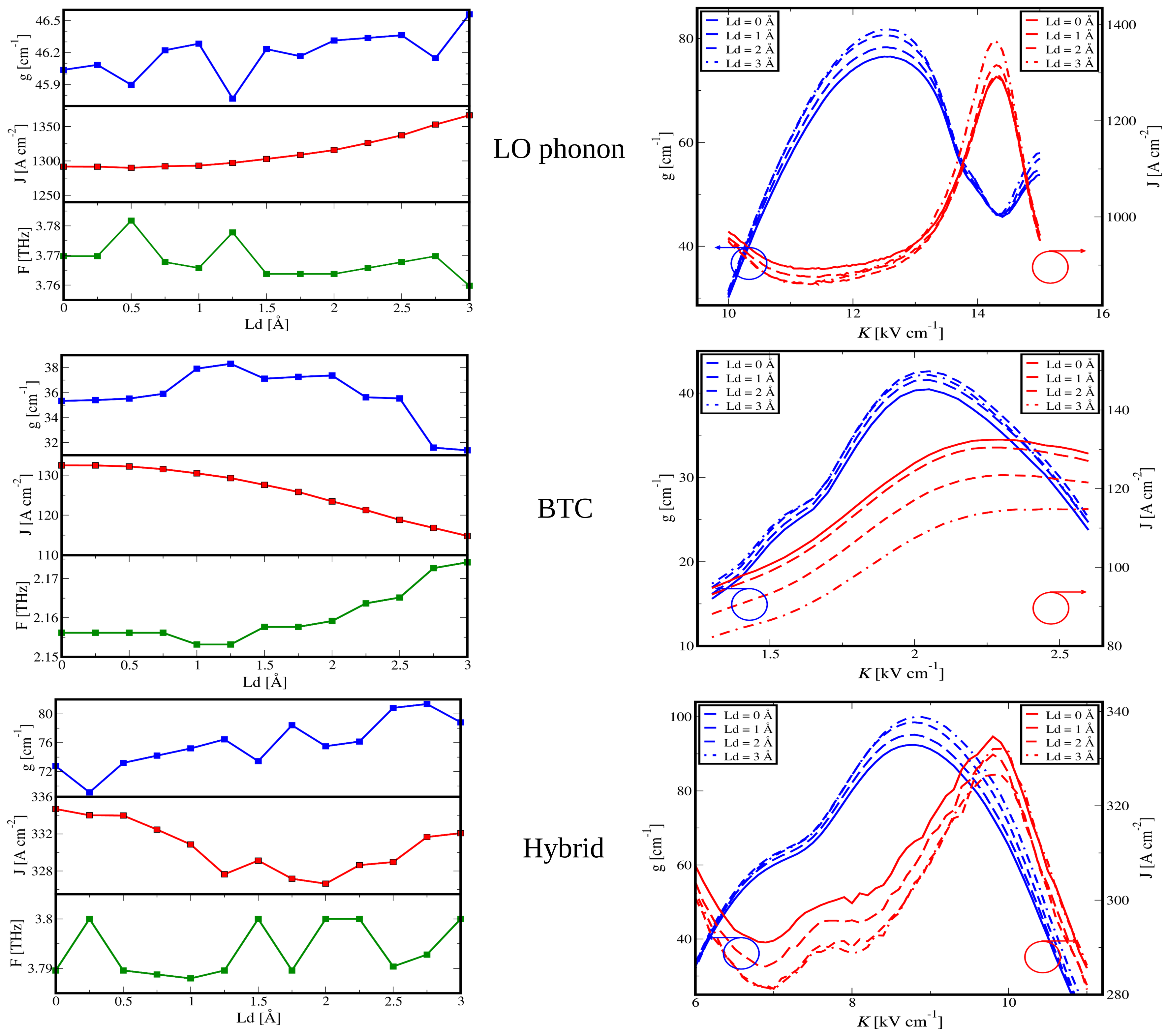
$$g=\frac{\omega}{cn_r}\mathrm{Im}\{\chi_{opt}\}=\frac{en_{2D}\omega}{cn_r\varepsilon_0A_0L_p}Tr\left(\rho^{ac+}Z\right)$$

3. Results

We apply our diffusion model to one of each design stated above:



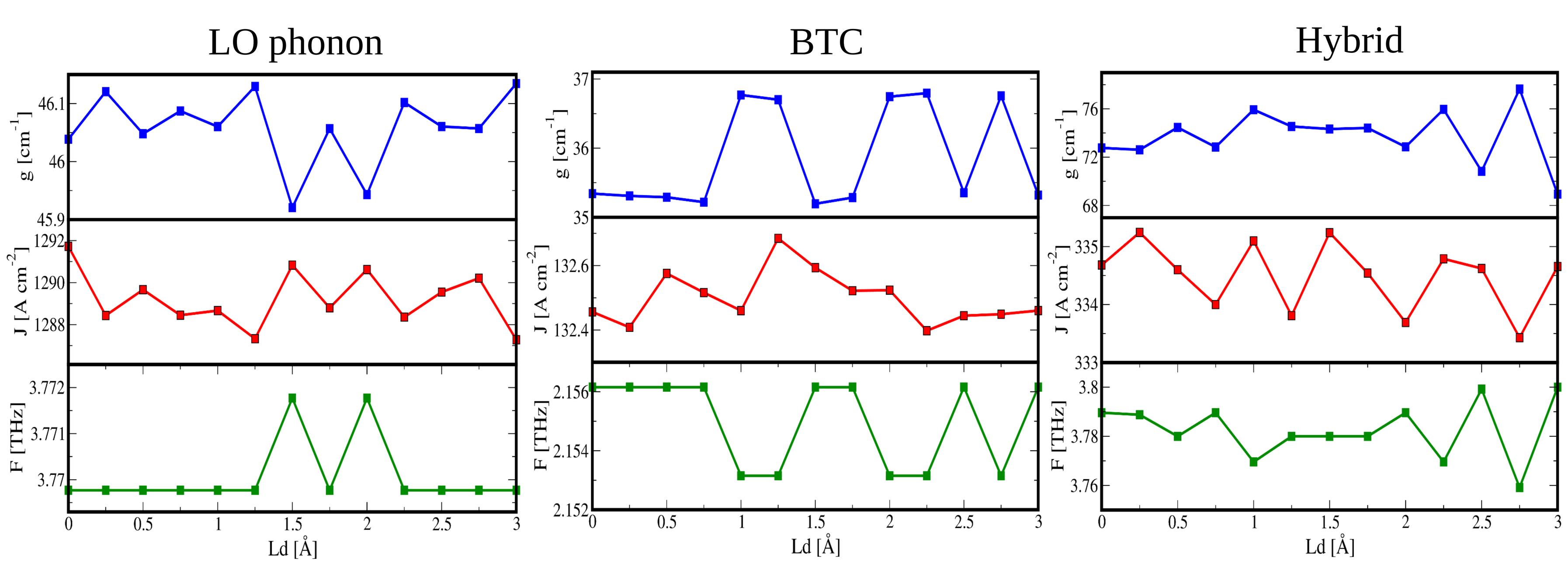
The LO phonon QCL achieved pulsed operation at high temperature 200K [5]. The lower laser level (LLL1) is efficiently depopulated by longitudinal optical phonon scattering into the injection laser level (ILL), that is located at a LO phonon energy (36 meV in GaAs) bellow the LLL1 and that is strongly coupled to the upper laser level (ULL) of the next period. Resonant tunneling occurs through the injection barrier depopulating the ILL.



Effect of interface diffusion on transport parameters in NDR point (left), and on material gain and current density versus external bias (right) in a LO phonon, BTC and Hybrid design QCL

The BTC QCL is designed for operation at a frequency of 2THz [4]. Extraction from the LLL to the ILL is achieved through diagonal transitions within the mini band, while the ILL is within the mini band and is strongly coupled to the ULL of the next period.

The Hybrid QCL is designed for record power emission [6]. The LLL is located in the top of the mini band, which allows fast electron extraction. The middle of the mini band is located 36 meV above the ILL, which is the LO phonon energy in GaAs.



The NDR point transport parameters are calculated for different values of diffusion length of the doping segregation and presented for all three laser designs.

4. Conclusion

This contribution shows that the inclusion of interface composition diffusion of the QCL structure has an important effect on modeling of the transport and significantly changes the material gain and current density, while for the same diffusion lengths used for interface composition diffusion doping segregation does not significantly effect QCL transport characteristics

References

[1]. J. Faist, et al., Science 264, 553-556 (1994).
[2]. B. S. Williams, Nature photonics, vol. 1, no. 9, p. 517 (2007).
[3]. Li Wang, et al., Appl. Phys. Express 16, 032007 (2023).
[4]. A. Demić, et al., IEEE Transactions on Terahertz Science and Technology, vol. 7, 368-377 (2017).
[5]. S. Fathololoumi, et al., Opt. Express, vol. 20, no. 4, pp. 3866–3876, (2012).
[6]. L. Li, et al., Electronics letters, vol. 50, no. 4, pp. 309–311, (2014).

Acknowledgements

This work was financially supported by the Vlatacom Institute of High Technologies under project 178, the Ministry of Science, Technological Development and Innovation of the Republic of Serbia under contract number: 451-03-47/2023-01/200103, "Multi-Scale Modeling of Terahertz Quantum Cascade Laser Active Regions", Multilateral scientific and technological cooperation in the Danube region 2020-2021, "DEMETRA: Development of high-performance mid-IR / THz quantum cascade lasers for advanced applications", Science Fund of the Republic of Serbia, Serbian Science and Diaspora Collaboration Programme: Knowledge Exchange Vouchers, and European Cooperation in Science and Technology (COST) Action CA21159 PhoBioS.