

# Performance comparison of terahertz quantum cascade lasers predicted by non-equilibrium Green's function method

H. Yasuda<sup>1,2</sup>, T. Kubis<sup>3</sup>, P. Vogl<sup>3</sup>, N. Sekine<sup>2</sup>, I. Hosako<sup>2</sup>, and K. Hirakawa<sup>1</sup>

<sup>1</sup>Institute of Industrial Science and Institute for Nano Quantum Information Electronics, University of Tokyo  
4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan  
Phone: +81-3-5452-6261, E-mail: [yasuda@nict.go.jp](mailto:yasuda@nict.go.jp)

<sup>2</sup>National Institute of Information and Communications Technology  
4-2-1, Nukui-Kitamachi, Koganei, Tokyo 184-8795, Japan  
<sup>3</sup>Walter Schottky Institute, Technische Universität München  
Am Coulombwall 3, 85748 Garching, Germany

## 1. Introduction

Remarkable progress in terahertz quantum cascade lasers (THz-QCLs) has been made since their first demonstration in 2002 [1]. However, operation of THz-QCLs at room temperature has not yet been realized. Recently, our group and Yamanishi et al. proposed novel designs of THz-QCLs, called “the four-level (4L) scheme”, which promises a much higher gain than the phonon-depopulation (RP) designs of a three-level scheme [2,3]. The 4L scheme intends to improve electron injection to the upper lasing level, utilizing an additional subband level. Yamanishi et al. reported an operation of the “indirect-pump” 4L QCL at 8  $\mu\text{m}$  [3]. The characteristic temperature  $T_0$  of 303 K of this laser is the highest among the reported QCLs.

## 2. Simulation results for THz-QCLs

We have calculated the performance of the 4L THz-QCL and the standard RP THz-QCL [4] with the non-equilibrium Green's function (NEGF) method. Figure 1 shows a flowchart of our NEGF program. Figure 2 shows the spectral functions, that is, the density of states with the in-plane wave vector  $k||=0$  and the conduction band diagrams of the RP and indirect-pump 4L THz-QCLs. In the conventional RP design given in Fig. 2(a), the upper lasing level (labeled as 3) is aligned with the injector state and is filled with electrons resonantly tunneled from the injector state. In contrast, in the indirect-pump 4L QCL of Fig. 2(b), electrons are injected to the additional level 4 and scattered from level 4 to the upper lasing level 3 by emission of longitudinal optical (LO) phonons. No resonant tunneling contributes to the filling of the upper lasing level.

Figure 3 shows the calculated local absorption coefficients of the RP and indirect-pump 4L THz-QCLs as a function of position and photon energy at 40 K. The local optical gain is observed mainly in the two wells defined as the active region. The maximum local gain of  $73 \text{ cm}^{-1}$  of the 4L QCL is an order of magnitude higher than that of the conventional RP QCL ( $\sim 10 \text{ cm}^{-1}$ ). The total gain over one period of the indirect-pump 4L QCL of  $14 \text{ cm}^{-1}$  is significantly larger than that of the RP QCL of  $4 \text{ cm}^{-1}$ . Figure 4 shows the energy-resolved electron distributions and the spectrum functions averaged over one QCL period of the QCLs at 40 K. The NEGF calculations indicate that the

origin of the larger terahertz gain is that almost all electrons accumulate in the upper lasing level 3 in the active region of the indirect-pump 4L QCL, as shown in Fig. 4(c), while only one half of the electrons are populated in the level 3 in the active region for the case of the RP QCL in Fig. 4(a).

The indirect-pump 4L QCL may be a good candidate for room-temperature operation in the THz frequency range. However, the NEGF calculations at 200K revealed that the maximum local gain of the indirect-pump 4L QCL decreases to  $5 \text{ cm}^{-1}$ , while that of the RP QCL is  $3 \text{ cm}^{-1}$ . We found that the main origin for the gain reduction is the thermally activated phonon scattering, where electrons in the upper lasing level acquire sufficient in-plane kinetic energy to emit an LO-phonon and relax to the lower lasing level in a non-radiative manner.

One candidate to suppress the influence of thermally activated phonon scattering is the application of high magnetic fields to quench the lateral motion of electrons or the use of material systems with larger LO phonon energies.

## 3. Conclusions

We have calculated performance of the novel four-level THz-QCL with the NEGF method. The calculation results for 40 K showed that the indirect-pump QCL has a larger THz gain. The main origin for this is that almost all electrons contribute to lasing in the new scheme. However, the advantage of gain deteriorates at 200 K due to thermally activated phonon scattering.

## References

- [1] R. Köhler, A. Tredicucci, F. Beltram, H. E. Beere, E. H. Linfield, A. G. Davies, D. A. Ritchie, R. C. Iotti, and F. Rossi, Nature (London) vol. 417, p. 156 (2002).
- [2] N. Sekine and K. Hirakawa, Japan Patent Application, P2006-181502 (2006).
- [3] M. Yamanishi, K. Fujita, T. Edamura, and H. Kan, Opt. Exp., vol. 16, p. 20748 (2008).
- [4] A. Benz, G. Fasching, A. M. Andrews, M. Martl, K. Unterreiner, T. Roch, W. Schrenk, S. Golka, and G. Strasser, Appl. Phys. Lett. vol. 90, 101107 (2007).

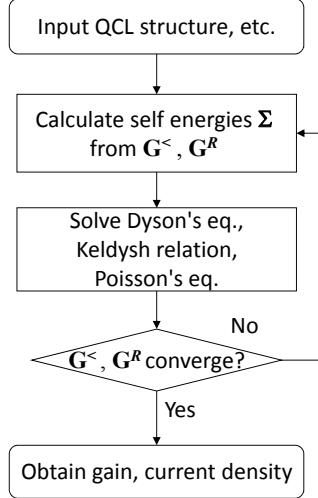


Fig. 1 Flowchart of our NEGF program.

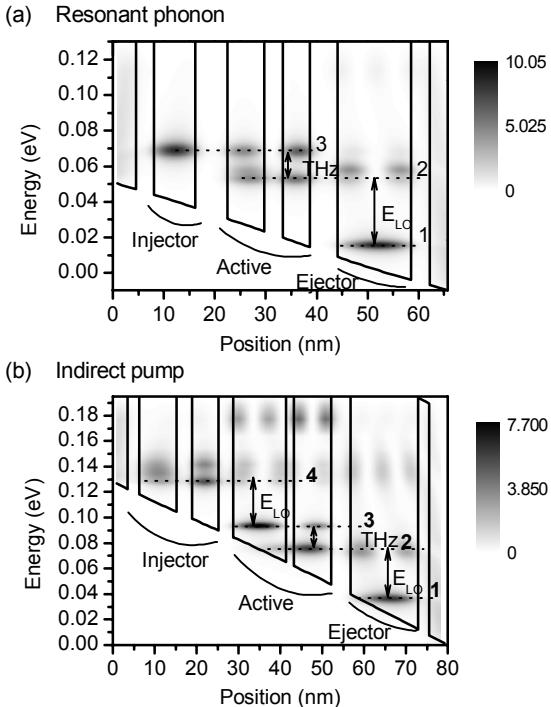


Fig. 2 Spectral functions and conduction band schematics of (a) the RP-QCL and (b) the indirect-pump 4L QCL.

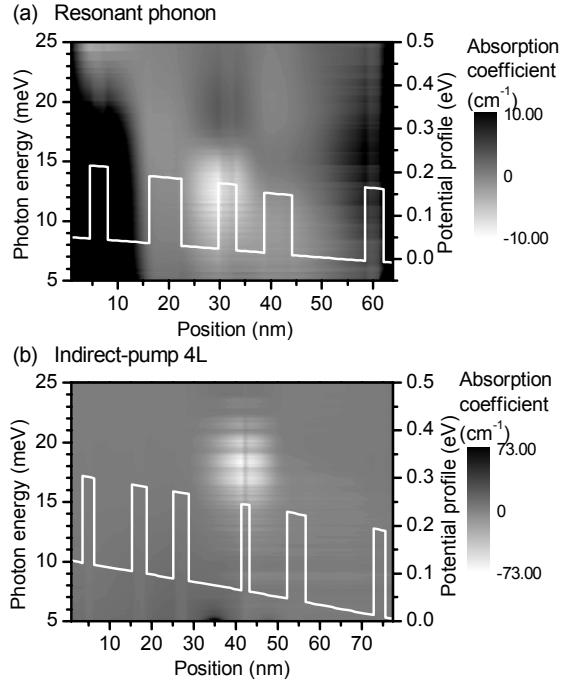


Fig. 3 Absorption coefficients as a function of position and photon energy of (a) the RP-QCL and (b) the indirect-pump 4L QCL at 40 K.

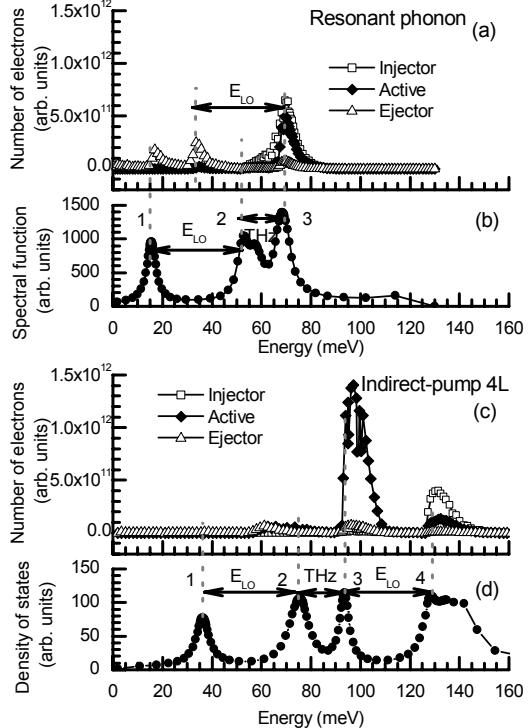


Fig. 4 Energy-resolved electron distributions in the injector, active, and ejector regions and spectral functions at 40K of (a)(b) the RP-QCL and (c)(d) the indirect-pump 4L QCL.