

# **Optimization of self-consistent approach for quantum cascade laser using shooting method and particle swarm optimization**

Yuankun Sun<sup>1,2</sup>, Peng Feng<sup>1</sup>, Haijun Zhou<sup>1</sup>, Weiling Chen<sup>3</sup>, Xin Li<sup>3</sup>, Liang Gong<sup>3a)</sup>, Biao Wei<sup>1</sup>, and Chen Peng<sup>2</sup>

Abstract We present a numerical optimization approach to simulate the output characteristics of a mid-infrared quantum cascade laser, taking into account the effect of subband electron temperature ( $T_{ei}$ ). The shooting method is used to simplify the calculation. The results give accurate subband electron temperatures when the external electric field is above the threshold. The results of the calculations are consistent with experimental results, thereby confirming that consideration of the subband electron temperature can improve our understanding of quantum cascade lasers and help guide future experimental work.

Keywords: quantum cascade laser, shooting method, infrared, electron temperature

Classification: Integrated optoelectronics

## 1. Introduction

Mid-infrared (MIR) lasers are in great demand for a variety of applications, including molecular spectroscopy, gas detection, medical diagnostics, chemical sensing, free-space communication [1, 2, 3, 4, 5], and numerous related applications. Quantum cascade lasers (QCLs) introduced in 1994 [6], have become important coherent MIR sources because of their high power, narrow linewidth, and roomtemperature operation [7]. To better understand and predict the behaviour of QCLs, numerical investigations have become a valuable tool. For example, numerical studies have been useful for predicting and analysing the carrier dynamics in quantum devices, and have contributed significantly to improving their design [8, 9]. In addition, the self-consistent energy balance (SCEB) model [10] has been shown to predict the lasing characteristics of QCLs without the computational demands of Monte Carlo [11] (MC) or non-equilibrium Green's function [12] (NGF) methods. The charge transport through a quantum cascade laser is thought to be mainly caused by incoherent electron-longitudinal optical phonon (LO) and electron-electron scattering [13]. The LO-phonon scattering in two-phonon reso-

a) gongl16@qq.com

DOI: 10.1587/elex.16.20190651 Received October 25, 2019 Accepted November 20, 2019 Publicized December 13, 2019 Copyedited January 10, 2020 nant QCL design is dominant [14]. To improve the accuracy of numerical simulation of QCLs, many parameters must be taken into account, such as the carrier temperature and optical emission. However, this proposition leads to a complicated multi-parameter SCEB model, which is prohibitively expensive computational. Therefore, the algorithm of the SCEB model needs to be improved.

In SCEB models, the carrier temperature includes the electron temperature [15] and the lattice temperature [16], with the former expected to be significantly greater than the latter [17]. Previous research has compared a SCEB model that considers the average electron temperature with one that considers the multi-subband electron temperature. However, most of them use the common method-dichotomy method. If we use this method to calculate the electron temperature of every energy level, although accurate results can be obtained, it will be very time consuming [18, 28]. Therefore, we need a better method to calculate the electron temperature of every energy level. The first step in the SCEB model is to solve the Schrödinger equation, for which several approaches are possible [20, 21, 22]. The transfer matrix approach can make solving the Schrödinger equation become a standard eigenvalue problem. However, some erroneous energy levels may be obtained that are not in the given quantum well, so these must be removed artificially. Besides, this approach is computationally expensive. An alternate method is the shooting method [22], which is arguably the simplest technique for solving this problem. The shooting method is simple, flexible, and versatile, and is easy to implement on a computer. The particle swarm optimization (PSO) algorithm starts from a random solution and obtains the optimal solution after several iterations. This parallel algorithm offers high precision and can optimize multiple parameters simultaneously, giving it a broad potential for simulating QCLs.

In this work, we propose an optimized model to determine the temperature of electrons in the conduction subbands and present the associated algorithm. The simulation tool determines the electron temperature of each subband for given external electric fields. The shooting method is used to calculate the subband wave functions, which significantly reduces the calculation time, and the particle swarm optimization algorithm is applied to investigate the subband electron temperature of a QCL, which significantly improves the accuracy of QCL simulations. Meanwhile, this optimized model allows for simultaneous optimization of multiple QCL parameters, which facilitates the development of self-designed QCL applications.

<sup>&</sup>lt;sup>1</sup>Key Laboratory of Optoelectronic Technology & Systems, Ministry of Education, Chongqing University, Chongqing 400044, China

<sup>&</sup>lt;sup>2</sup>China Academy of Engineering Physics, Mianyang 621000, China

<sup>&</sup>lt;sup>3</sup>Department of Respiratory and Critical Care Medicine, The First Affiliated Hospital, Army Medical University, Chongqing 400038, China

### 2. Numerical approach

The simulation is based on the well-known  $1\frac{1}{2}$ -period model developed by K. Donovan et al. [23, 24]. As shown in Fig. 2, the active region is sandwiched between two injection regions. The simulation model includes both spontaneous emission and stimulated emission. The electron distribution of each subband can be described by a Fermi-Dirac function. The electron temperature Tei describes the electron Fermi distribution in each subband. In addition, the optical emission affects the electron distribution of each subband, and the electron distribution of each subband is closely related to the electron temperature of the given subband. We thus need to consider how optical emission affects the QCL characteristics, which means that we must solve the full laser rate equations in the SCEB model to obtain QCL characteristics. The full laser rate equations are

$$\frac{\mathrm{d}n_{i}}{\mathrm{d}t} = -n_{i} \sum_{k \neq i} \frac{1}{\tau_{i,k}} + \sum_{k \neq i} \frac{n_{k}}{\tau_{k,i}}; \ i \neq \text{upper, lower}$$
(1)

$$\frac{dn_{upper}}{dt} = -n_{upper} \sum_{k \neq upper} \frac{1}{\tau_{upper,k}} + \sum_{k \neq upper} \frac{n_k}{\tau_{k,upper}} - S\Gamma_p \frac{c}{n_0} g_c(n_{upper} - n_{lower})$$
(2)

$$\frac{dn_{lower}}{dt} = -n_{lower} \sum_{k \neq lower} \frac{1}{\tau_{lower,k}} + \sum_{k \neq lower} \frac{n_k}{\tau_{k,lower}} + S\Gamma_p \frac{c}{n_0} g_c(n_{upper} - n_{lower})$$
(3)

$$\frac{dS}{dt} = S \left[ N_p \Gamma_p \frac{c}{n_0} g_c (n_{upper} - n_{lower}) - \frac{c}{n_0} \alpha \right] + N_p \beta \frac{n_{upper}}{\tau_{cp}}$$
(4)

Eq. (1)–(4) are for non-lasing subbands, the upper laser subband, the lower laser subband, and the photon emission, respectively. For convenience, we refer to Eq. (1)–(3) as the partial-rate-equations (PREs) and to Eq. (1)–(4) as the full-rate-equations (FREs). The stimulated emission rate between subband i and f can be derived from the Fermi's golden rule (25):

$$R_{fi} = S \frac{c}{n_0} g_c = \frac{2\pi}{\hbar} \frac{e^2 E_0^2}{4m^{*2} \omega^2} |\langle f| \hat{e}. \vec{p} |i\rangle|^2 \delta(E_f^0 - E_i^0 - \hbar \omega)$$
(5)

The spontaneous emission rate is given by

$$\frac{1}{\tau_{\rm sp}} = \frac{e^2 n_0 \omega^3}{3\pi \varepsilon c^3 \hbar} |\langle \mathbf{f} | \mathbf{z} | \mathbf{i} \rangle|^2 \tag{6}$$

The first step in SCEB model is to solve the Schrödinger equation, which determines the energy levels in the quantum well structure [27]. In previous research [18, 19], we used the transfer matrix approach in our simulation, which transforms the Schrödinger equation into a standard eigenvalue problem. The eigenvalues and eigenvectors of the transfer matrix correspond to the energy levels and wave functions of the QCL, respectively. However, the transfer matrix approach [20, 21, 22, 23] yields all mathematical solutions, some of which may not be physical; that is, their energy levels place the electrons outside of the quantum well. In this case, we have to artificially remove the erroneous energy levels. And, this approach is computationally expensive. The energy levels in the quantum well structure must satisfy the Schrödinger equation

$$\left[-\hbar^2 \frac{\mathrm{d}}{\mathrm{d}z} \left(\frac{1}{2\mathrm{m}^*(\mathrm{E},\mathrm{z})} \frac{\mathrm{d}}{\mathrm{d}z}\right) + \mathrm{V}(\mathrm{z})\right] \varphi_\mathrm{n}(\mathrm{z}) = \mathrm{E}_\mathrm{n}(0)\varphi_\mathrm{n}(\mathrm{z}) \quad (7)$$

where the effective mass  $m^*(E, z)$  is not constant (unlike the case of parabolic bands) but in fact accounts for band non-parabolicity [30, 31, 32, 33] through its energy dependence

$$m^{*}(E, z) = m^{*}(0, z)[1 + \alpha(E - V)]$$
(8)

where the parameter  $\alpha$  is a constant, as defined in reference (33).

The shooting method [26] converts Eq. (7) into a finite difference equation. In this method, the first derivative is approximated as:  $\partial_z \psi(z_n + \delta z) \approx \frac{\psi(z + \delta z) - \psi(z - \delta z)}{2\delta z}$ . Hence the second derivative as:  $\partial_z^2 \psi(z_n + \delta z) \approx \frac{\psi(z + 2\delta z) - 2\psi(z) + \psi(z - 2\delta z)}{(2\delta z)^2}$ , where  $\delta z$  is a small displacement. The finite difference representation of the second derivative may then be simplified by substituting  $\delta z$  for  $2\delta z$ :  $\partial_z^2 \psi(z_n + \delta z) \approx \frac{\psi(z + \delta z) - 2\psi(z) + \psi(z - \delta z)}{(\delta z)^2}$ . Using this form for the second derivative ative in the original Schrödinger Eq. (7), we obtain

$$\psi(z + \delta z) - 2\psi(z) + \psi(z - \delta z)$$
$$= \frac{2m^*(E, z)}{\hbar^2} (\delta z)^2 [V(z) - E] \psi(z)$$
(9)

which implies that, if the wave function is known at the two points  $(z - \delta z)$  and z, then the value of the wave function at  $(z + \delta z)$  can be calculated for any energy E. This method is known as the shooting method. Using two known values of the wave function  $\varphi(z - \delta z)$  and  $\varphi(z)$ , a third value  $\varphi(z + \delta z)$  can be predicted. In the same way, using this new point  $\varphi(z + \delta z)$ , together with  $\varphi(z)$ , a fourth point  $\varphi(z + 2\delta z)$ , can be calculated, and so on. Hence the complete wave function can be deduced for any particular energy. The first two values of the wave function can be deduced based on simple symmetry arguments. Numerically, these eigenenergies are found by using standard techniques such as the Newton-Raphson iteration. The method searches all solutions within a selected range, so it does not get solutions outside the quantum well. In other words, no manual filtering is required.

The second step in the SCEB model is to solve the PREs and the FREs to study the characteristics of QCLs. In order to take the subband electron temperature into account, the energy balance method developed by Harrison [29, 34] is used to determine the effective subband electron temperature  $T_{ei}$ . In the steady state, the total kinetic energy of electrons in a QCL remains unchanged. Conservation of energy requires  $E_f^{(0)} + E_f(k_f) = E_i^{(0)+E_i(k_i)\pm E_{phonen}}$ , where positive (+) sign is used for phonon emission and the negative (-) sign for phonon absorption. Applying conservation of energy to each subband can give a different electron temperature for each subband, as shown by following equation:

$$\frac{d[\delta E(k)]}{dt} = \sum_{i} \sum_{f} \sum_{k_{i}} \left[ \frac{n_{i}(k_{i}, T_{ei})}{\tau_{if}^{ems}(k_{i}, T_{ei})} (E_{i}^{(0)} - E_{f}^{(0)} - E_{f}^{(0)} - E_{phonon}) + \frac{n_{i}(k_{i}, T_{ei})}{\tau_{if}^{abs}(k_{i}, T_{ei})} (E_{i}^{0} - E_{f}^{0} + E_{phonon}) \right]$$
$$= 0$$
(10)

The summation in Eq. (10) only includes the phononelectron scattering, which greatly simplifies the calculation of the subband electron temperature T<sub>ei</sub>.

Our simulation uses 100, 150, 200 particles to optimize the electron temperature in the SCEB model. Each particle has seven dimensions corresponding to the subbands. The search space (i.e., the electron temperature range) is 30-600 K, and the velocity range is 1-25 K, which determines the speed and direction of the particles. The initial position and velocity of each particle are assigned random in the search space. We substitute each particle into the loop simultaneously to calculate the electron distribution and scattering time, find the optimum value for each dimension according to the set conditions and record it for the next iteration. The velocity and position of each particle is updated in each iteration by using

$$v_{mn}^{k+1} = w \times v_{mn}^{k} + f_1 \xi(p_{nb}^k - x_{mn}^k) + f_2 \eta(g_{nb}^k - x_{mn}^k) \quad (11)$$

and the position of each particle is updated by using

$$\mathbf{x}_{mn}^{k+1} = \mathbf{x}_{mn}^{k} + v_{mn}^{k+1} \tag{12}$$

After several iterations, we obtain the optimized electron temperature of each subband. Table I defines the relevant variables and parameters for Eq. (1)-(12).

To obtain the electron temperature of each subband, we propose the algorithm shown in Fig. 1. First, we form a closed loop to solve the Schrödinger equation to obtain the subband wave functions and the corresponding subband edge energies, we then calculate the potential due to the resulting charge distribution, add it to the original bandedge potential, and then solve the Schrödinger equation again. The process is repeated until the energy eigenvalues converge. At this point, the wave functions are simultaneously solutions to both the Schrödinger equation and Poisson's equation. We then set the lattice temperature TL, the electric field strength E, and some other parameters. After initializing the particles of T<sub>ei</sub>, we obtain the scattering time and electron distribution of each subband by solving the PREs. Note that these results are not modified.

The energy conservation is applied to each subband to determine the optimal value of each dimension of the particle, and other particles are moved the optimal value of each dimension at a certain speed and direction. The optimal electron temperature of each subband is updated in each iteration. Finally, after several iterations, we obtain the optimal electron temperature, the scattering time, and the electron distribution of each subband. Since the PSO is a parallel algorithm, as long as the particles and judgment conditions are set properly, the optimal electron temperature of each subband can be found simultaneously within several iterations.

Table I. V	anables and parameters in Eq. $(1)$ – $(12)$ .
Symbol	Definition
n <sub>i</sub>	Electron population in subband $ i\rangle$
$ au_{i,k}$	Average electron-phonon scattering time for transition from subband $ i\rangle$ to subband $ k\rangle$
S	Photon population
$\Gamma_{\rm p}$	Optical waveguide confinement factor
c	Speed of the light in the vacuum
n <sub>0</sub>	Waveguide core refractive factor
gc	Optical gain cross section
N <sub>p</sub>	Number of stages
α	Total optical loss
β	Fraction of spontaneous photons emitted into the lasing mode
$1/\tau_{ m sp}$	Spontaneous emission rate
upper	Upper laser subband
lower	Lower laser subband
e	Unit charge
E <sub>0</sub>	Electrical field
ω	Photon angular frequency
$\vec{p}$	Momentum operator
ê	Polarization of the electrical field
ħ	Planck's constant divided by $2\pi$
E <sub>i</sub> <sup>(0)</sup>	Subband edge of the subband $ i\rangle$
3	Material permittivity
φ	Wave function
Е	Eigenenergy
n	Energy quantum number
E <sub>phonon</sub>	Phonon energy
k <sub>i</sub>	Electron wave vector in subband $ i\rangle$
$n_i(k_i)$	Electron population at $k_i$ in subband $ i\rangle$
$\tau_{if}^{ems(abs)}(k_i,T_{ei})$	Electron transition rate from $k_i$ state of subband $ i\rangle$ to subband $ f\rangle$ by phonon emission (absorption)
$v_{ m mn}^{ m k}$	Electron temperature variation velocity of the m particle of n dimension
$\mathbf{f}_1$	Self-cognition coefficient, weight coefficient of particle tracking their historical optimal values
$f_2$	Society-cognition coefficient, weight coefficient of optimal value of particle tracking group
$\xi, \eta$	Random numbers
$p_{nb}^k$	Optimal solution for n dimensions
$g^k_{nb}$	Optimal solution for all particles in n dimensions
x <sup>k</sup> <sub>mn</sub>	Position in dimension n of particle m in iteration k

#### 3. Simulation and experiment

We simulate a standard 35-stage In<sub>0.52</sub>Al<sub>0.48</sub>As/In<sub>0.53</sub>-Ga<sub>0.47</sub>As type-I four-level Fabry-Perot QCL based on the two-phonon resonant design with a laser cavity length of 1.358 mm [35]. The effective electron sheet density is about  $20.4 \times 10^{10}$ , and we assume that all dopants are ionized. We use Harrison's method to calculate the tunnelling effect from the injection level to the upper laser level [23]. The total optical loss is assumed to be  $23.3 \text{ cm}^{-1}$ , including 14.3 cm<sup>-1</sup> waveguide loss [35] and 9 cm<sup>-1</sup> mirror loss for waveguide refractive index of 3.4 [36].



Fig. 1. The algorithm to obtain the electron temperature of each subband (with energy balance indeed)

Fig. 2 gives, for a bias electrical field of 40 kV/cm, the calculated electrical potential and the spatial probability distribution of each subband in the active region and in the two injection regions. Each region contains seven confined subbands. Energy levels A3 and A4 are the lower and upper laser level, respectively, and the band gap between them is 159 meV, which corresponds to the QCL central wavelength of 7.81 µm, (i.e., the wavelength given in Ref. [35]).



Fig. 2. Calculated conduction subbands and the moduli squared of the relevant wavefunctions for an external electric field of  $40 \, kV/cm$ .

By using the algorithms described in Fig. 1, at a lattice temperature of 300 K, we simulate the QCL for extern electric field: 41 kV/cm, which corresponds to above the threshold electric field. We obtain the electron temperature of each subband. The electron temperature of each subband affects the lifetime of the electron state, so it also affects the optical gain of the laser.

As shown in Fig. 3, we obtain the electron temperature of each subband separately. The inset (a) of Fig. 3 shows the relaxation time of every subband. The relaxation time of the A4 subband is more than twice that of the A3 subband relaxation time, indicating the population inversion is formed at the upper laser level and the lower laser level. The inset (b) of Fig. 3 shows the relationship between the optical gain and the injection current density (including optical emission) for  $T_e = T_{ei}$  and  $T_e \neq T_{ei}$ . When the number of iterations and the number of particles change, we always get almost the same electron temperature of each subband. With the QCL in stable operation, the change of electron temperature is a dynamic equilibrium progress. When the external electric field is below the threshold, the electron temperatures of subbands A1 and A4 are higher than those of the other subbands because electrons are stimulated to subband A<sub>4</sub> by the external electric fields, but there is no optical radiation output. Most of the energy transfer goes into promoting electrons from the ground state to the high-k state through intraband transitions, which increases the electron temperature.

We mainly discuss the electron temperature of A1 to A4. From the inset (a) of Fig. 3, we can know that the relaxation time of A1 is much larger than that of A2 and A3, but their electron temperatures are not much different. This is mainly because the electron temperature not only reflects the electron distribution but also reflects the state of the electron. The low electron temperature of A4 is mainly due to its low-k state. However, electron-phonon scattering can lead to electrons transferring from subband A<sub>3</sub> to subband A<sub>2</sub>, which decreases the electron temperature of subband A<sub>3</sub>. Similarly, electron-phonon scattering can lead to electrons transferring from subband A2 to subband A1, which decreases (increases) the electron temperature of subband  $A_2$  (A<sub>1</sub>). A small number of electrons occupy subbands  $A_5-A_7$ , so the electron temperature of  $A_5-A_7$ does not rise appreciably.



Fig. 3. Electron temperature of each subband above the threshold, 100(50) means the simulation contain 100 particles and 50 iterations, and so on. The inset (a) shows the relaxation time of every subband. The inset (b) shows that comparison of optical gain for Te = Tei and  $Te \neq Tei$  at different injection-current densities.

When the external electric field is below the threshold, the electron temperature of each subband increases as the external electric field increases. This trend remains unchanged because, as the external electric field increases and the QCL emits no radiation, the energy input increases and is mostly converted to thermal energy, which increases the electron temperature. Once the external electric field exceeds the threshold, the QCL begins to emit radiation, and most of the electrons of the upper laser subband transfer back to the ground state, releasing thermal energy in the form of optical radiation. Thus, the electron temperature of subband  $A_4$  decreases sharply. Because no other effective channel exists to release energy, the electron temperature of other subbands remains high.

Inclusion of the subband electron temperature in the simulation leads a decrease in the optical gain of the QCL before the laser gain is saturated. Compared with the case in which all subbands have the same electron temperature, the effect of assigning the appropriate specific electron temperature to each subband leads to an increase in the threshold current density of about  $0.44 \text{ kA/cm}^2$ .



Fig. 4. The I-V characteristics of simulation (two methods) and experiment.

As shown in Fig. 4, we obtain the QCL simulation (two methods) and experimental I-V curves, which have the same trend. And when the simulation applying the shooting method, their difference is smaller, with only about 45 mA of difference being found. Although the QCL I-V curves of the simulation (two methods) and experiment have the same trend, there is still a difference between the measured and simulated optical emission power because of the loss of optical transition and the conversion efficiency of detection elements. We also find that, when considering the electron temperature of each subband and applying the shooting method, the simulation results accurately estimate the QCL characteristics.

## 4. Conclusion

To conclude, we present herein an optimized model to investigate the output characteristics of QCLs, taking into account the effects of subband electron temperature. This model allows us to study how subband electron temperature effects laser performance. We can change the electron distribution, and in particular the electron distribution in the lasing subband. In addition, the shooting method is applied to simplify the calculation. Finally, considering the electron temperature of each subband and applying the shooting method, the simulation results can be obtained faster and more accurately. This model also simultaneously optimizes multiple QCL parameters, which facilitates the development of self-designed QCL applications.

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#### References

- S. Borri, *et al.*: "Frequency modulation spectroscopy by means of quantum cascade laser," Appl. Phys. B **85** (2006) 223 (DOI: 10.1007/s00340-006-2343-6).
- [2] C. Peng, et al.: "High-speed mid-infrared frequency modulation spectroscopy based on quantum cascade laser," IEEE Photon. Technol. Lett. 28 (2016) 1727 (DOI: 10.1109/LPT.2016.2554359).
- [3] C. Roller: "Nitric oxide breath testing by tunable-diode laser absorption spectroscopy: Application in monitoring respiratory inflammation," Appl. Opt. 41 (2002) 6018 (DOI: 10.1364/AO. 41.006018).
- [4] F. Capasso: "Quantum cascade lasers: Ultrahigh-speed operation optical wireless communication narrow linewidth and far-infrared emission," IEEE J. Quantum Electron. 38 (2002) 511 (DOI: 10. 1109/JQE.2002.1005403).
- [5] R. Martini: "High-speed modulation and free-space optical audio/ video transmission using quantum cascade lasers," Electron. Lett. 37 (2001) 191 (DOI: 10.1049/el:20010102).
- [6] J. Faist, et al.: "Quantum cascade laser," Science 264 (1994) 553 (DOI: 10.1126/science.264.5158.553).
- [7] R. F. Curl, *et al.*: "Quantum cascade lasers in chemical physics," Chem. Phys. Lett. **487** (2010) 1 (DOI: 10.1016/j.cplett.2009. 12.073).
- [8] R. C. Iotti and F. Rossi: "Microscopic modelling of opto-electronic quantum devices: A predictive simulation tool," J. Comput. Electron. 2 (2003) 191 (DOI: 10.1023/B:JCEL.0000011423.43254.57).
- [9] R. C. Iotti and F. Rossi: "Microscopic modelling of semiconductorbased quantum devices: A predictive simulation strategy," Phys. Status Solidi B 238 (2003) 462 (DOI: 10.1002/pssb.200303163).
- [10] G. Chen, et al.: "Self-consistent approach for quantum cascade laser characteristic simulation," IEEE J. Quantum Electron. 47 (2011) 1086 (DOI: 10.1109/JQE.2011.2153827).
- [11] R. C. Iotti and F. Rossi: "Carrier thermalization versus phononassisted relaxation in quantum-cascade lasers: A Monte Carlo approach," Appl. Phys. Lett. **78** (2001) 2902 (DOI: 10.1063/1. 1370537).
- [12] S.-C. Lee and A. Wacker: "Nonequilibrium greens function theory for transport and gain properties of quantum cascade structures," Phys. Rev. B 66 (2002) 245314 (DOI: 10.1103/PhysRevB.66. 245314).
- [13] R. C. Iotti and F. Rossi: "Nature of charge transport in quantumcascade lasers," Phys. Rev. Lett. 87 (2001) 146603 (DOI: 10.1103/ PhysRevLett.87.146603).
- [14] C. Jirauschek and T. Kubis: "Modeling techniques for quantum cascade lasers," Appl. Phys. Rev. 1 (2014) 011307 (DOI: 10.1063/ 1.4863665).
- [15] It should be noted that this temperature Tei has nothing to do with the effective temperature invoked in a macroscopic n-level description, which becomes negative in the case of population inversion.
- [16] P. Harrison: "The nature of the electron distribution functions in quantum cascade lasers," Appl. Phys. Lett. **75** (1999) 2800 (DOI: 10.1063/1.125154).
- [17] D. Indjin, *et al.*: "Self-consistent scattering model of carrier dynamics in GaAs-AlGaAs terahertz quantum-cascade lasers," IEEE Photon. Technol. Lett. **15** (2003) 15 (DOI: 10.1109/LPT. 2002.805801).
- [18] C. Peng, et al.: "Numerical study of subband electron temperature effect on a mid-infrared quantum cascade laser output characteristics," Semicond. Sci. Technol. 28 (2013) 105008 (DOI: 10.1088/ 0268-1242/28/10/105008).
- [19] C. Peng, *et al.*: "Investigation of subband electron temperatures of quantum cascade lasers," IEEE Photon. J. **11** (2019) 1500710 (DOI: 10.1109/JPHOT.2019.2896081).
- [20] B. Jonsson and S. T. Eng: "Solving the Schrodinger equation in

arbitrary quantum-well potential profiles using the transfer matrix method," IEEE J. Quantum Electron. **26** (1990) 2025 (DOI: 10. 1109/3.62122).

- [21] C. Jirauschek: "Accuracy of transfer matrix approaches for solving the effective mass Schrödinger equation," IEEE J. Quantum Electron. 45 (2009) 1059 (DOI: 10.1109/JQE.2009.2020998).
- [22] Y. Ando and T. Itoh: "Calculation of transmission tunneling current across arbitrary potential barriers," J. Appl. Phys. 61 (1987) 1497 (DOI: 10.1063/1.338082).
- [23] E. Cassan: "On the reduction of direct tunneling leakage through ultrathin gate oxides by a one-dimensional Schrodinger-Poisson solver," J. Appl. Phys. 87 (2000) 7931 (DOI: 10.1063/1.373477).
- [24] P. S. J. Zory: Quantum Well Lasers (Academic Press Inc, 1993).
- [25] S. L. Chuang: *Physics of Optoelectronic Devices* (Joh Wiley & Sons Inc, New York, 1995).
- [26] P. Harrison: Quantum Wells, Wires and Dots: Theoretical and Computational Physics of Semiconductor Nanostructures (Wiley-Interscience, 2005).
- [27] K. Donovan, et al.: "Self-consistent solutions to the intersubband rate equations in quantum cascade lasers: Analysis of a GaAs/ AlxGa1-xAs device," J. Appl. Phys. 89 (2001) 3084 (DOI: 10. 1063/1.1341216).
- [28] D. Indjin, *et al.*: "Self-consistent scattering theory of transport and output characteristics of quantum cascade lasers," J. Appl. Phys. **91** (2002) 9019 (DOI: 10.1063/1.1474613).
- [29] P. Harrison, *et al.*: "Electron temperature and mechanisms of hot carrier generation in quantum cascade lasers," J. Appl. Phys. **92** (2002) 6921 (DOI: 10.1063/1.1517747).
- [30] X. Gao, et al.: "X-valley leakage in GaAs/AlGaAs quantum cascade lasers," Appl. Phys. Lett. 89 (2006) 191119 (DOI: 10. 1063/1.2387485).
- [31] X. Gao, et al.: "X-valley leakage in GaAs-based midinfrared quantum cascade lasers: A Monte Carlo study," J. Appl. Phys. 101 (2007) 063101 (DOI: 10.1063/1.2711153).
- [32] X. Gao, *et al.*: "Design and simulation of deep-well GaAs-based quantum cascade lasers for 6.7 μm room-temperature operation," J. Appl. Phys. **102** (2007) 113107 (DOI: 10.1063/1.2820039).
- [33] G. Liu and S.-L. Chuang: "Modeling of Sb-based type-II quantum cascade lasers," Phys. Rev. B 65 (2002) 165220 (DOI: 10.1103/ PhysRevB.65.165220).
- [34] H. Asai and Y. Kawamura: "Intersubband absorption in In<sub>0.53</sub>-Ga<sub>0.47</sub>As/In<sub>0.52</sub>Al<sub>0.48</sub>As multiple quantum-wells," Phys. Rev. B 43 (1991) 4748 (DOI: 10.1103/PhysRevB.43.4748).
- [35] Z. Liu, *et al.*: "Room-temperature continuous-wave quantum cascade lasers grown by MOCVD without lateral regrowth," IEEE Photon. Technol. Lett. **18** (2006) 1347 (DOI: 10.1109/LPT.2006. 877006).
- [36] M. Levinshtein, et al.: Handbook Series on Semiconductor Parameters, Ternary and Quaternary III–V Compounds, vol. 2 (World Scientific, Singapore, 1999).