Simulation of quantum cascade lasers – optimizing laser performance

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The commercialization of quantum cascade lasers (QCLs) has just begun. Their emission wavelengths depend on the specific cascade layer sequence the lasers consist of. Simulations of the physical processes in QCLs allow for the product-specific optimization of emitted wavelengths and output performance.

The semiconductor band gap of the individual layers of quantum cascade lasers has no influence on the emission wavelength. This offers the opportunity to develop lasers in the mid (3–30 µm) and far infrared (30–500 µm) spectral region. The far infrared region is also known as the terahertz region (0.6–10 THz). Already theoretically predicted in 1971 [1], QCLs had not been realized until 1994 at Bell Laboratories (USA) [2]. Typically, QCLs are grown by epitaxial methods such as molecular beam epitaxy. Layers of different semiconductor materials – each only a few atomic layers thin (1–15 nm) – are deposited onto a thin slice of a semiconductor crystal (**figure 1**), e.g. InAlAs/InGaAs layers on InP wafers. The sequence of the layers, their widths and materials are chosen such that the electronic wave functions are optimized with respect to energy and probability distribution (wave function engineering). This guarantees laser emission at the desired frequency with the highest possible power. State-of-the-art output power at room temperature for continuous operation lies in the range of 50–300 mW and about twice as high in pulsed mode operation.

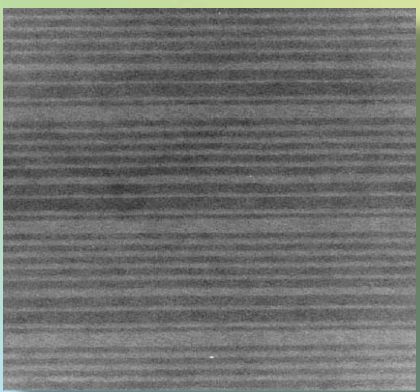


Figure 1:* *Transmission electron microscopy photograph of the active zone of a QCL (approx. 3 periods). The layers of AlGaAs (bright) and GaAs (dark) have a width of between 2 and 6 nm *(J. Raabe, Universität Regensburg)*

Market survey

Currently, quantum cascade lasers form a niche market. For a couple of years, QCLs have been available from several small start-ups such as Alpes Lasers (Neuchâtel/Switzerland) and nanoplus (Würzburg/Germany). Larger companies such as Alcatel-Thales (France) and Hamamatsu (Japan) have commenced QCL business only recently. Today, Alpes Lasers, a spin-off of the University of Neuchâtel, is the market leader with a market share of about 80%. Actually, one of their founders, Prof. Jérôme Faist, is one of the inventors of the quantum cascade laser.

Depending on the wavelength and performance characteristics, the price per unit for QCLs ranges from approximately 5000 to 20 000 €. By contrast, other types of semiconductor laser, such as the VCSELs

Originally published in German in Photonik 1/2008

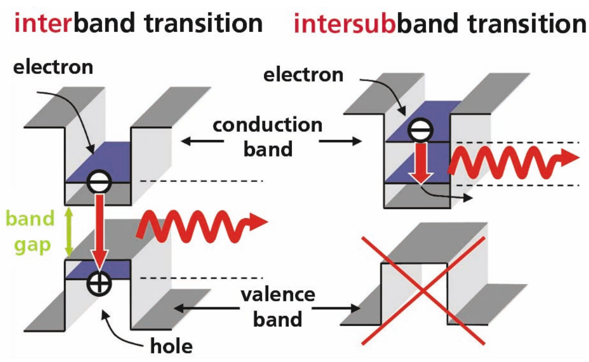


***Figure 2:** Interband (conventional semiconductor laser) vs. intersubband transition (QCL). The emitted wavelength of the QCL is independent of the band gap of the material and only depends on the thicknesses of the layers* *(after G. Scarpa, TU München)*

(vertical cavity surface emitting laser) built into computer mice are available at around 0.40 € per unit.
At present, annual sales for QCLs are estimated to reach 1000 units. The forecast for 2010 is around 100 000 units at prices of about 200–300 €/unit for standard lasers. The opportunities of this market have been recognized by further start-ups such as Maxion Technologies (Maryland/USA, a spin-off of the US Army Research Laboratory), Q-on (Vienna/Austria, a spin-off of the Vienna University of Technology) or Argos Tech (Santa Clara/USA, a continuation of the former QCL activities of Agilent Technologies). Measurement equipment that utilizes QCLs is meanwhile available, e.g. from neoplas control from Greifswald (Germany), Cascade Technologies (Scotland) or Daylight Solutions (USA). Currently, applications can be identified principally in the field of gas sensor systems (wavelength range 4–12 µm). Using the TILDAS technique (tunable infrared laser diode absorption spectroscopy) molecules such as CO, CO_2, CH_4, NH_3, N_2O, SO_2, O_3, HNO_3, etc. can be detected with high spectral resolution, thus enabling measurement of their concentrations quantitatively in real time. Although QCLs compete with lead salt lasers in this wavelength range, they do have fundamental advantages, such as room temperature operation. To date, terahertz QCLs have not been successfully operated at room temperature. However, this would be most desirable in order to unlock the large potential in the area of security screening as THz radiation can pass through clothing but does not penetrate metal objects. Intensive work and effort is also being put into the realization of QCLs based on the silicon-germanium material system as these would be compatible with conventional CMOS technology.

Operation principles of a quantum cascade laser

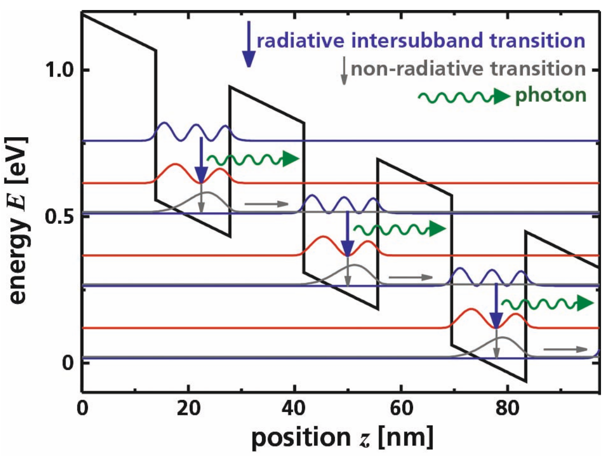
In conventional quantum well lasers, photons are generated by the recombination of electrons and holes (interband transitions). Hence, the laser wavelength predominantly depends on the band gap of the associated semiconductor materials.
By contrast, the photons in QCLs are generated by intersubband transitions, i.e. transitions within the conduction band, and the wavelength of QCLs is thus independent of the material's band gap (**figure 2**). The emission wavelength of QCLs actually depends on the choice of layer properties and can be varied in a certain range (mid and far infrared or THz regime, respectively). It is also typical of QCLs that the current is mediated by only one sort of charge carrier (either electrons or holes) instead of both kinds as is the case for example in quantum well lasers. Consequently, complicated many-body effects such as excitons (electron-hole pairs) play no role in QCLs.
It is common to use the Schrödinger equation as an idealized model for QCLs:

$$\left(-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m_e(z)}\frac{\partial}{\partial z}+E_c(z)\right)\psi_n(z)=E_n\psi_n(z) \quad (1)$$

Here, m_e is the material dependent effective electron mass, E_c represents the conduction band edge (including the electric field) and $\hbar$ is the reduced Planck's constant. By solving this equation, one obtains the energies E_n (eigenvalues) and the wave functions ψ_n (eigenfunctions) of the n electron states. **Figure 3** shows the probability density of the electrons for a simple quantum cascade structure, obtained by the nextnano³ software[1]. This simple structure consists of three quantum wells and is tilted by a constant electric field that corresponds to the applied bias. In any one period, an electron falls to the ground state by a combination of radiative and non-radiative decay. However, as this ground state (grey) is energetically aligned

[1] A demo version of the nextnano³ software with this QCL structure as an example can be downloaded from www.nextnano.de/customer/download.php

***Figure 3:** Conduction band profile of a quantum cascade structure at an electric field strength of 89 kV/cm and corresponding wave functions of the electron states (ψ^2). In order to induce efficient tunnelling, the lowest state of each quantum well is resonant with the upper state of the neighbouring, energetically lower, quantum well*



with the upper state (blue) in the neighbouring period, the electron then quantum mechanically tunnels into this period. Through a succession of such steps, the electron thus cascades down through the structure (moving left to right in the figure), emitting a photon for each period. Typically, around 30–200 periods are used in a QCL device.

A fundamental property of every laser is a pronounced population inversion, i.e. the occupation of the upper state has to exceed the number of electrons in a lower state significantly. For efficient laser operation, it is also essential that the radiative rate of relaxation from the upper state is greater than that occurring through thermal emission of phonons. nextnano^3 also derives the relevant optical transition probabilities from the wave functions. Variations of materials, quantum well and barrier thicknesses, as well as of the applied electric fields allow one to tune the population inversion, transition probabilities and emission spectra, and to customize QCL performance.

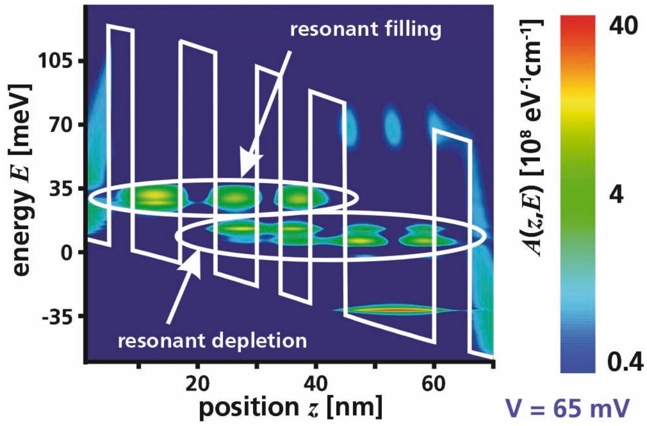


***Figure 4:** Contour plot of the calculated energy resolved local density of states $A(z,E)$ as a function of position z and energy E. The white line represents the self-consistently calculated conduction band profile. The applied bias is 65 mV. The resonant filling and depletion of the lasing states (centre) is clearly visible*

Realistic modeling of quantum cascade lasers

The solution of the one-dimensional Schrödinger equation is numerically very efficient and therefore best suited to yield a rough estimate of the QCL properties. Unfortunately, electronic transport in QCLs is much more complicated and the one-dimensional model is highly oversimplified. A QCL is made of many layers of various semiconductor materials. Therefore, electrons are not limited to a one-dimensional motion parallel to the applied electric field, but they can also propagate within the layers, i.e. perpendicular to the electric field. These additional degrees of freedom result in a continuous energy spectrum instead of a discrete one (E_n in Eq. (1)). Furthermore, no device constructed of semiconductor layers is free from impurity atoms or imperfections at the interfaces between the layers. These "defects" cause significant (position dependent) deviations of the QCL from the idealized representation in Eq. (1). At finite temperatures, even perfect devices contain periodic lattice vibrations (phonons) at which electrons frequently scatter and suffer significant broadening in the energy spectrum.

All of these aspects can be successfully modelled by the non-equilibrium Green's function method (NEGF) that was simultaneously developed by the US scientists Schwinger, Kadanoff and Baym as well as the Russian scientist Keldysh in the 1960s. Instead of discrete results (figure 3), this method yields maxima of the electronic probability density (local density of states) that are broadened in energy and position. This can be seen in **figure 4** which shows a contour plot of the energy resolved local density of states for the case of the active region of an AlGaAs/GaAs THz QCL during laser operation. The white solid line depicts the conduction band profile $E_c(z)$. In comparison with the results of the Schrödinger equation, the realistic width (with respect to energy) of the states in NEGF calculations softens the alignment conditions for the resonant filling of the upper laser state and the resonant depletion of the lower laser state. Consequently, only realistic calculations reveal the actual voltage range within which QCLs can operate.

Important information of QCL characteristics can also be deduced from the electron density, i.e. the occupation of the laser states. Unlike the simplified model, the NEGF method allows for a

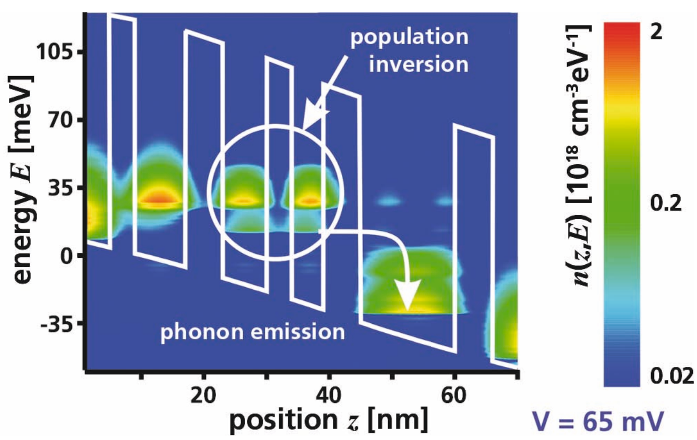


***Figure 5:** Contour plot of the calculated energy resolved electron density $n(z,E)$. The population inversion of the electronic states in the central double quantum well is clearly visible: The upper laser level has a higher density than the lower one, which is efficiently emptied by resonant phonon emission (arrow)*

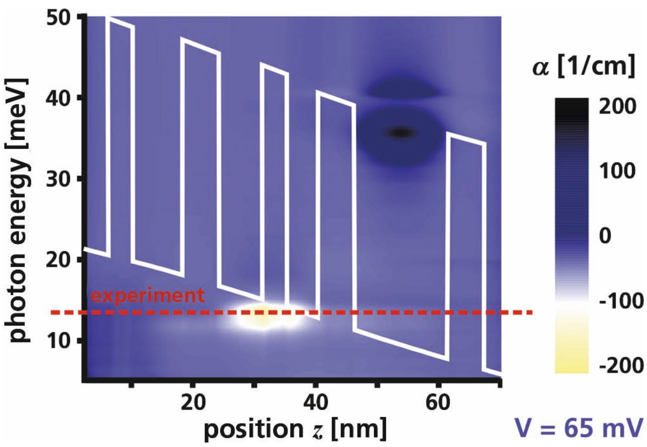


***Figure 6:** Contour plot of the calculated absorption coefficient $\alpha(z,\hbar\omega)$ as a function of position z and photon energy $\hbar\omega$. The red line indicates the measured emission line of the QCL. The conduction band profile (white) is only meant as a guide to the eye*

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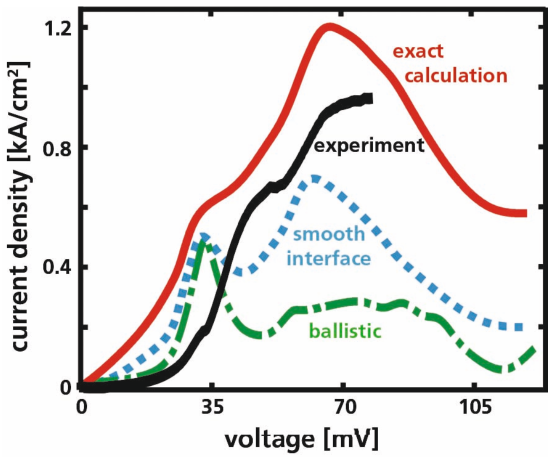

***Figure 7:** Current-voltage characteristics of the THz QCL at a temperature of 100 K. The exact calculation (red) is close to the experiment of Ref. [4] (black) whereas the calculation with smooth interfaces (blue) and the ballistic calculation (i.e. all scattering mechanisms are neglected, green) deviate strongly*

consistent determination of the state occupation [3]. **Figure 5** depicts a contour plot of the energy (E) and spatially (z) resolved electron density of the situation in figure 4. A pronounced population inversion, i.e. a higher occupation of energetically higher states is clearly visible in the centre of the device. Consequently, the electrons can scatter into the lower laser level by emission of photons and thus amplify the optical laser field there. This is accentuated in **figure 6**, which shows the calculated optical absorption coefficient of the same situation as a function of the growth coordinate z and the photon energy. The absorption coefficient is negative at the position of the population inversion. Consequently, more photons are emitted than absorbed. This leads to a positive gain in the bright region indicated in figure 6. The dotted line corresponds to the measured wavelength of the laser and agrees very well with the calculated gain.

Furthermore, the current-voltage characteristics predicted by this method also show good agreement with experiment. **Figure 7** compares the measured current density (black) with results of the NEGF calculations (simulation: current through 1 period, experiment: current through 175 periods). One can clearly see that only the exact calculation that takes into account all relevant scattering mechanisms (red curve) agrees well with experiment [4]. Calculations that assume ideal smooth interfaces (blue), or a device that is completely free from imperfections (ballistic curve in green) deviate qualitatively from experiment. Rather rough interfaces have been included in the calculations (represented by the red curve) in order to emphasize the difference with calculations that are based on smooth interfaces. Results with a realistic roughness lie between these extreme cases. During laser operation, the device is heated significantly beyond the heat sink temperature of 5 K. Since the exact device temperature is extremely difficult to assess experimentally, a constant temperature of 100 K has been assumed. Each bias point takes about one day of computational time.

In conclusion, the NEGF method provides experimentally inaccessible information (figures 4, 5 and 6) that is vital for a deeper understanding of the device physics. This allows for predictions of device characteristics and facilitates customer-oriented device design.

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