Design of THz Quantum Cascade Lasers by Simulations

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An approach is described for designing a terahertz quantum cascade laser based on AlGaAs-GaAs. Parameters such as doping concentration, which are independent of the frequency are optimally chosen. The remaining parameters are varied in order to obtain the right frequency at the best high temperature and oscillatory strength. Simulations are suitable for quantum cascade lasers structure, mainly, for calculation for its energy diagram, emission frequency, oscillatory strength and dipole moment of radiative transition. The emission of 3.5 THz is estimated based on a three-well resonant-phonon.

Keywords: Qauntum cascade lasers, THz lasers, low temperature physics, microwave & far infrared, resonant-phonon, remote sensing in the space.

There have been enormous progress and changes in the development of quantum cascade laser during the last decade, however, it was initially proposed by Kazarinov & Suris [5] in 1971. It was only in 2001, that terahertz quantum cascade laser (QCL) was realized for the first time [6]. This one emitted at a frequency of 4.4 THz. So far, the terahertz quantum cascade lasers designed operated at a low temperature of 225 K in 2009 [8]. It remains a challenge to produce emission in the domain of THz. Recently, it has been shown that such an emission is possible at room temperature [7].

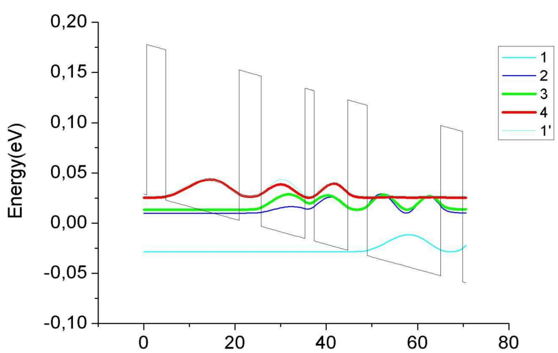

FIG. 1: Showing resonant-phonon energy for the three wells [1].

The main part of designing a quantum cascade laser is how to choose number of wells in each module and the grid points for the quantum well as well as barrier. The operating temperature for THz QCL could be as low as 25 K because, at a low temperature, the disturbance due to thermal oscillations is less.

The choice of these factors is how to make a compromise. The main part of the simulations is based on quantum mechanical calculation, i.e., wave functions, using the Nextnano software [1]. The multiband Schrödinger

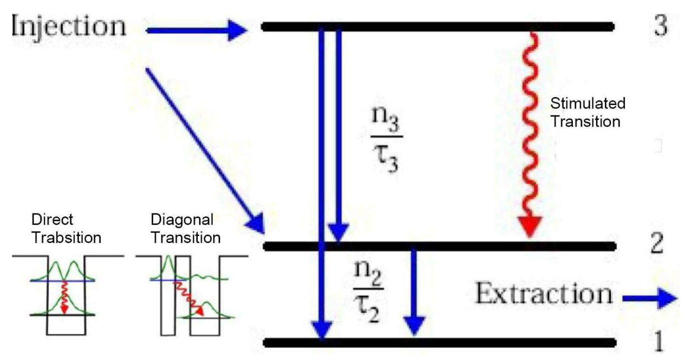

FIG. 2: Depiction of main transitions involved in quantum cascade lasers.

and Poisson equations are solved self consistently. There are mainly two steps involved:

1) The potential is adjusted correspondingly while Fermi levels of the electrons and holes are kept fixed.

2) The potential is held fixed and Fermi levels are calculated by using current equation.

The calculated values of the Fermi levels are used to adjust the potential. Furthermore, the calculated potential value is used to find out new Femi levels, ultimately converging to the final solution, so-called self-consistent.

The software has a vast variety of examples and 'input files' (commands) which could be modified for further development. Figure 3 and Fig. 4 ((by Nexnano) are showing good match with each other. Mainly, there are three kind of quantum cascade laser design, namely: Chirped superlattice, bound-to-continuum and resonant phonon design (Fig. 1) which is very well described in [4]. It describes one of the first phonon resonant design. Herein, the tunnelling of the phonon is exploited. Nextnano is also capable of calculating gain, however, it can take at least one day with a semi-super computer. Evidently, the material, amount of doping (well or barrier), thicknes of the lasing well play crucial role but easy to make an optimal choice. One of the device consists of GaAs/$Al_{0.15}$ $Ga_{0.85}$As layers with thicknesses (nm, starting from the injector barrier) **4.8**/8.5/**2.8**/8.5/**4.2**/16.4, with the barriers in bold fonts. The extraction barrier is doped to n = 3.0 * 10^{10} and applied bias is 12.5 kV/cm.

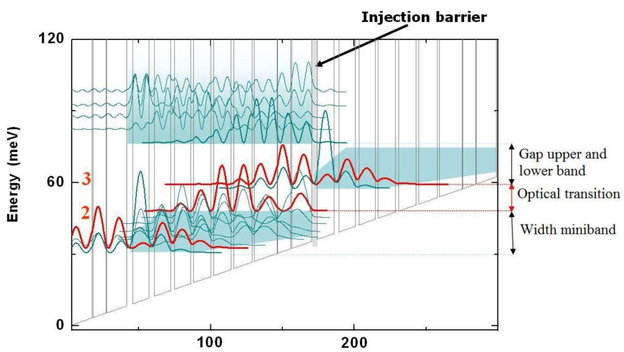

FIG. 3: Bound-to-continuum design diagram according to [2].

The simulation of quantum cascade laser remains challenging. Nextnano is a suitable software but it is rather tedious. The shape of the wave function calculated by Nextnano match well with other groups , as showm in Fig. 3 and Fig. 4. It is also compatible with the measured radiative energy by other groups. Room-temperature emission at THz requires needs additional innovation by designing a new active region. And through the use of new material, for example, the GaN-AlGaN system because its large LO-phonon energy (about 90 meV) [3] which is needed to avoid thermally activated phonon. It remains to be an open question.

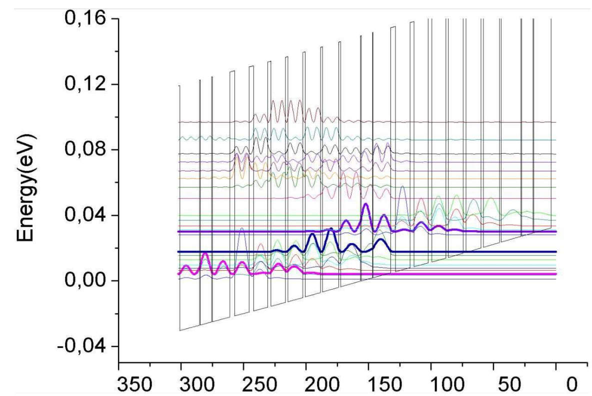

FIG. 4: Bound-to-continuum design diagram according to 'nextnano' [1].

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