Theoretical simulation of quantum cascade lasers based on InGaAs/AlInAs and InGaAs/AlAsSb quantum wells

K A Romanova and Y G Galyametdinov
Kazan National Research Technological University, 68 Karl Marx Street, Kazan, 420015, Russia
E-mail: ksenuya@mail.ru

Abstract. Quantum cascade lasers based on semiconductor InGaAs/AlInAs and InGaAs/AlAsSb quantum wells exhibit electronic intersubband transitions within conduction bands and attract much attention due to their operation at room-temperature short wavelengths. In this work we performed a theoretical simulation of such quantum cascade lasers and studied the influence of their construction and application conditions on optical behaviour. The intersubband absorption processes in these quantum well structures were studied. Electronic properties and the conduction band edge profiles were simulated as well as the probability densities of the Wannier-Stark states were determined. The simulation results showed that with the rise of the temperature the threshold current density increases which also leads to a decrease in the optical gain. An increase of the applied electric field is accompanied by the optical gain rising and decrease of the threshold current density that results in a blue shift of laser frequency.

1. Introduction
Intersubband transitions in semiconductor materials with quantum wells attract increasing attention due to their advanced application in optical switches for communication networks, quantum cascade lasers (QCLs), terahertz photodetectors, gas sensor systems. QCL represents a compact and coherent source wherein the optical transition can be tuned by creating an active layer with multiple quantum wells. The unique emissive characteristics of QCLs determine their promising application in medicine, environmental monitoring, safety control and communication. Their wavelength range includes the mid-IR (3-25 μm) and terahertz region of the electromagnetic spectrum (300 GHz-10 THz). For the mid-IR region they are the only semiconductor lasers that operate at room temperature. Some of them may be applied as single-mode radiation sources with the opportunity of tuning the laser generation wavelength. The terahertz QCLs are one of the few solid-state sources of coherent electromagnetic radiation with milliwatt power in the frequency range of 2-5 THz [1-3].

Nowadays most studies of QCLs are focused on the enhancement of their radiation power and decrease of the laser threshold current along with the modification of their design. They consist of several layers of semiconductor materials with a thickness of few atomic layers on a thin sample of semiconductor crystal. The variation of semiconductor materials, sequence of the layers and their width allows to modify laser power and emission at the required frequency. The process of double phonon resonance gives a significant population inversion due to the several quantum wells and states in the active region of the laser that differ by the value of the phonon energy. The active region may
also include interminiband transitions in chirped superlattices or bound-to-continuum transitions of electrons between states localized close to the injection barrier and a miniband that results in an increase in laser power, a decrease in threshold current and large gains in a wider frequency range.

Computer simulation methods allow one to select the most convenient components for effective optoelectronic devices as well as to predict optical behavior of compounds and output performance characteristics of devices before their experimental implementation [4, 5]. Materials with remarkable conduction band offsets (the quantum well depth between the barrier and the quantum well materials) at the heterogeneous junction can be used for effective optoelectronic devices and QCLs. For example, InGaAs/AlAsSb system has a conduction band offset around 1.6 eV [6]. Therefore, in this paper, we theoretically studied the performance of QCLs based on InGaAs/AlInAs and InGaAs/AlAsSb semiconductor materials using simulation methods. The conduction band edge profiles, wave functions of transitions and probability densities of the Wannier-Stark states were simulated. Based on the obtained results the effectiveness of QCLs based on these substances was estimated and the opportunities of theoretical simulation of QCLs and their optical behavior were investigated.

2. Computational technique

The characteristics of InGaAs/AlInAs and InGaAs/AlAsSb QCLs were simulated using the nextnano software [7] and non-equilibrium Green's function method (NEGF), which made it possible to obtain the conduction band edge profiles, wave functions for intersubband transitions and Wannier-Stark states. To confirm the accuracy of the calculations, a comparison of the calculated data with the literature was made [8-10]. Simulations were performed at different temperatures, values of the applied electric fields and component contents.

3. Results and discussion

Short wavelength intersubband transitions that occur in the conduction band of quantum wells can be characterized by relaxation times less than picoseconds, prominent transition dipole moments and beneficial low absorption saturation energy. The variation of QCL design and layer sequence allows to change the emission wavelength of such transitions. The principles of QCLs performance significantly differ from laser diodes or quantum well lasers based on semiconductor materials in which photon generation occurs due to the recombination of an electron and a hole. In quantum well lasers its wavelength is defined by the band gap of semiconductor materials. In QCLs electrons are the only charge carriers and photons are generated by intersubband transitions within the conduction band. Therefore, the emission wavelength of the QCL does not depend on the band gap of materials but is defined by the choice of layer properties (material, sequence, width) and can be changed in a certain range. Photons emitted during laser operation are generated during quantum transitions of an electron between different energy levels inside a quantum well. These levels are formed artificially as a result of creating an active region from ultrathin layers of semiconductor materials. The resulting active region represents a superlattice that includes a series of alternate nanometer potential barriers and quantum wells. The observed splitting of the conduction band into allowed and forbidden subbands (minibands) can be explained by the superposition of the periodic potential of the superlattice and the crystal field potential. As a result, the movement of electrons is carried out within the given minibands perpendicular to the layer interface. The electron energy in such quantum wells is determined by the width of the well and the height of the potential barrier between neighboring wells.

Laser generation can be disturbed due to the leakage of electrons due to their tunneling to the states that form a wide quasicontinuum that reduces the population of the upper energy level. In order to avoid this process an injector or a superlattice with a low density of states is added to the QCL before the subsequent cascade. It should not include resonance states energetically coinciding with the upper level of the quantum well, but its main electronic level should correspond to the upper level in the next well. This injector forms a mini-gap that blocks transitions from the upper laser level and the injection of electrons occurs due to resonant tunneling that unites the active zones.
In QCLs, unlike other lasers, the electron remains in the conduction band after the emission of a photon, since its generation occurs due to the transition between energy levels in the quantum well. Then the electron can sequentially move to the identical neighboring active region, where another photon can be emitted, etc. A similar effect of photon cascade emission can be achieved by alternation of active regions with doped ones into which electrons are injected. As a result, such a cascade represents an energy ladder, with electrons movement along the steps and emission of photons on each of the stages-cascades. The resulting quantum efficiency of the cascade effect observed during laser operation exceeds unity and leads to a significant radiation power of the device as compared to laser diodes.

Consequently, QCL is a multilayer heterostructure placed in a waveguide perpendicular to the layers wherethrough an electric current is passed. This multilayer structure contains alternating active regions, within the boundaries of which photon emission occurs, and injection regions, which act as quantum barriers through which electrons tunnel to the next region. When electron passes through each of the cascades an emission of a photon occurs, and many photons are received due to the transitions through the entire laser. Therefore, a larger number of cascades allow one to obtain more photons. An increase of the number of cascades allows a significant increase in the output power of the device and a decrease in the threshold generation current. The development of highly efficient QCLs can assume the presence of more than 40 cascades.

Studied lattice-matched semiconductor materials have a sufficient conduction band offsets: InGaAs/AlAsSb ~ 1.6 eV, InGaAs/AlInAs ~ 0.51 eV [5, 11, 12]. As in the conduction band diagram (figure 1a) the X-valley of the barrier material AlAsSb locates below the Γ-valley the electron confinement can be reduced if the initial state of the laser transition will be above X-valley due to the X-Γ scattering. The solid and dashed lines on the figure 1a represent the Γ- and X-valley energy positions of materials respectively. The material of quantum well InGaAs has a lower position of X-valley in comparison with AlAsSb that restrain the application of QCLs in shorter wavelength region. Therefore, the location of the laser transition above the X-valley of InGaAs also leads to the electron loss. The wavy line represents the emission process due to the energy transition from the state that locales below the Γ-valley of InGaAs. Consequently, detailed study of photophysical features of QCLs is quite essential for the development of their improved implementations particularly for the cases of laser state locations below the X-valley of InGaAs.

![Figure 1](image)

**Figure 1.** Schematic (a) and calculated (b) conduction band diagram of the QCL based on InGaAs/AlAsSb system with the corresponding probability densities of the Wannier-Stark states.
The calculated conduction band edge profile and corresponding probability densities of the Wannier-Stark states of the QCL based on InGaAs/AlAsSb obtained as a result of the simulation in the nextnano program as one of the examples is shown on the figure 1b. The simulations were also carried out in the temperature range of 0-310 K and with the variation of electric fields of 0-200 kV/cm with different alloy compositions (x) of In$_{x}$Ga$_{1-x}$As, AlAs$_{x}$Sb$_{1-x}$ and Al$_x$In$_{1-x}$As. This figure presents a typical squarelike potential shape of intersubband transitions with energy separation of 0.8 eV as compared with 0.8 eV in 9 monolayer thick In$_{0.78}$Ga$_{0.22}$As [8]. According to the simulated data the thinning of the quantum well layer results in the decrease of this transition energy.

The slope of the conductivity dependence was less pronounced in comparison with other semiconductor lasers and cascade lasers with quantum wells. The threshold current density increases with a decrease in the applied electric field which coincides with experimental dependences [13]. The optical gain decreases with the increase of the temperature and the direct correlation with linear behavior are observed with the increase of applied electric field that shifts the emission wavelength to the shorter region. This can be explained by the temperature dependence of the Fermi-Dirac distribution of the electrons in quantum wells ground state and the different character of subbands in conduction band diagram.

The calculations performed for the systems with different compositions (x) of In$_{x}$Ga$_{1-x}$As, AlAs$_{x}$Sb$_{1-x}$ and Al$_x$In$_{1-x}$As showed that the increase of Al content in barrier material AllnAs above 50% lead to increase of the conduction band offset by more than 0.1 eV and to reduction of the band gap. A similar dependence is also observed with the decrease of Ga content below 45% in quantum well material InGaAs. When choosing AllnAs as the barrier material in comparison with AlAsSb more significant increase of the conduction band offset was noticed. The thickening of the quantum well can lead to the higher subband energy separations and as result to absorption at lower wavelengths. The observed data is similar to the experimental dependences obtained in [13]. Authors showed that by increasing the In content above 53% in InGaAs and reducing it below 52% in InAlAs, the conduction band offset can be increased.

The obtained difference between simulated results and literature data can be explained by interface defects, concentration heterogeneity, fluctuations and roughness in the experimental samples. In order to compensate such defects the additional layers are usually applied on the well-barrier interfaces. Since the change of In content also leads to the strain between layers (tensile in the barrier and compressive in quantum well) an active region that compensate strain can be obtained by appropriate layer thicknesses and material compositions.

4. Conclusion

Theoretical study of quantum cascade lasers based on InGaAs/AllnAs and InGaAs/AlAsSb semiconductor materials showed short wavelength intersubband transitions within conduction bands of quantum wells. The influence of the temperature, the value of the applied electric field and the composition of the materials on the optical behaviour of such devices was studied. Conduction band edge profiles, electronic properties and the probability densities of the Wannier-Stark states were simulated. The influence of the temperature and the values of the applied electric field on the threshold current density and the optical gain were revealed. According to the simulated data the temperature
and the threshold current density increase simultaneously leading to a decrease in optical gain. However the observed temperature dependence is not sufficiently pronounced. An increase in the optical gain can be obtained by the increase in the applied electric field which is also accompanied by the decrease in the threshold current density and a blue shift in the generation frequency. It follows from the obtained results that it is very promising to create QQLs. Therefore the study of QQLs characteristics can be carried out using numerical simulation methods as well as the design of devices with custom-oriented behaviour.

Acknowledgments
Financial support was provided by a grant from the Russian Science Foundation (project No. 18-73-00100). The calculations were performed using the facilities of the Joint Supercomputer Center of Russian Academy of Sciences and the Supercomputing Center of Lomonosov, Moscow State University [14].

References
[1] Dunn A et al. 2020 Nat. Commun. 11 835
[2] Curwen C A, Reno J L and Williams B S 2019 Nat. Photonics 13 855-9
[3] Jirauschek C and Kubis T 2014 Appl. Phys. Rev. 1 011307
[4] Romanova K A, Kremleva A V and Galyametdinov Y G 2019 Liq. Cryst. and their Appl. 19 15
[5] Polushin S G, Lezova I E, Polushina G E, Rogozhin V B, Ryumtsev E I, Romanova K A and Galyametdinov Y G 2018 JETP Letters 107 431-4
[6] Georgiev N and Mozume T 2001 J. Vac. Sci. Technol. B 19 1747-51
[7] Birner S, Hackenbuchner S, Sabathil M, Zandler G, Majewski J A, Andlauer T, Zibold T, Morschil R, Trellakis A and Vogl P 2006 Acta Phys. Pol. A 110 111-24
[8] Cristea P, Fedoryshyn Y, Holzman J F, Robin F, Jäckel H, Müller E and Faist J 2006 J. Appl. Phys. 100 116104
[9] Yang Q, Manz C, Bronner W, Köhler K and Wagner J 2006 Appl. Phys. Lett. 88 121127
[10] Giorgetta F R, Baumann E, Théron R, Pellaton M L, Hofstetter D, Fischer M and Faist J 2008 Appl. Phys. Lett. 92 121101
[11] Wadehra A, Nicklas J W and Wilkins J W 2010 Appl. Phys. Lett. 97 092119
[12] Zhang X H, Chua S J, Xu S J and Fan W J 1998 J. Appl. Phys. 83 5852-4
[13] Asgari A and Khorrami A A 2013 Opto-Electron. Rev. 21 147-52
[14] Voevodin V V, Zhumatiy S A, Sobolev S I, Antonov A S, Bryzgalov P A, Nikitenko D A, Stefanov K S and Voevodin V V 2012 Open Systems J. 7 36-9