

# Self-consistent design of strain-compensated InGaAs/InAlAs quantum cascade laser structures: towards short wavelengths

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**Abstract**—We designed  $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{In}_y\text{Al}_{1-y}\text{As}$  quantum cascade laser (QCL) structures, based on the four-quantum well active region operating at  $\lambda \sim 2.8\text{-}3.3 \mu\text{m}$  in terms of an objective function, i.e.,  $z_{UL}^2(1 - \tau_L/\tau_{UL})\tau_U$ , related to the optical gain, including dipole matrix element ( $z_{UL}$ ) and population inversion between electron transitions. For shorter wavelength emission, the higher conduction band discontinuity ( $\Delta E_c$ ) was achieved by changing the In mole fraction of  $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{In}_y\text{Al}_{1-y}\text{As}$  strain-compensated layers. The use of strain-compensated  $\text{In}_{0.72}\text{Ga}_{0.28}\text{As}/\text{In}_{0.3}\text{Al}_{0.7}\text{As}$  pair (i.e.,  $\Delta E_c = 857 \text{ meV}$ ) leads to the shortest wavelength up to  $\lambda \sim 2.84 \mu\text{m}$  with  $\tau_{43} = 3.96 \text{ ps}$ ,  $\tau_4 = 1.21 \text{ ps}$ ,  $\tau_3 = 0.55 \text{ ps}$  and  $z_{43} = 0.57 \text{ nm}$  under an electric field of  $94 \text{ kV/cm}$ .

## I. INTRODUCTION

The quantum cascade laser (QCL) based on intersubband transitions within the conduction band is the most promising mid-infrared semiconductor light source. The emission wavelength of QCLs depends on the thickness of layers and their composition which determine the electron wave functions of subbands under an applied electric field rather than the intrinsic bandgap of constituent materials, allowing for laser operation over a wide wavelength range of  $3.4\text{-}24 \mu\text{m}$ . The QCLs operating at short wavelength ( $3.4\text{-}4 \mu\text{m}$ ) have been demonstrated by using a larger conduction band discontinuity of strain-compensated structure. In 1998, a continuous-wave (CW) power of  $120 \text{ mW}$  at  $15 \text{ K}$  was reported at  $\lambda \sim 3.4 \mu\text{m}$  [1] and CW power of  $143 \text{ mW}$  at  $298 \text{ K}$  was demonstrated at  $\lambda \sim 3.8 \mu\text{m}$  [2]. The strain-compensated design, i.e., the compressive strain in the wells compensated by equal and opposite tensile strain in the barriers, reduces the current leakage and improves the performance of short-wavelength QCLs due to the increased conduction band discontinuity ( $\Delta E_c$ ) [3]. In this work, we report the design optimization of strain-compensated  $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{In}_y\text{Al}_{1-y}\text{As}$  QCL structures based on a four-level system for the shorter wavelength ( $\lambda \sim 2.8\text{-}3.3 \mu\text{m}$ ).

## II. SIMULATION AND DISCUSSION

In order to achieve the high device performance, the design of

active region/injector in QCLs is very important, requiring further optimization of layer structures. Thus, we used the self-consistent calculation algorithm of double infinite feedback (DIF) loops as shown in Fig. 1. For the criteria parameter related the modal optical gain, we define the figure (O) as objective function [4].

$$O = z_{UL}^2(1 - \tau_L/\tau_{UL})\tau_U, \quad (1)$$

where  $z_{UL}$  is the dipole matrix element between upper subband and lower subbands for optical transition and  $\tau_U$  and  $\tau_L$  are lifetimes of electron in each subband, respectively, and  $\tau_{UL}$  is the scattering time from upper level to lower level.

The first step for design is that the initial QCL structure with properly designed injector is to be numerically analyzed. And then, many QCL structures are created by regularly changing the first pair ( $n = 1$ ) of each quantum well and barrier in active region. For each changed QCL structure, the objective functions and emission wavelengths are calculated by solving one dimensional effective-mass Schrödinger equation for the potential profile of the structure. Among them, the QCLs structure having the lowest wavelength with objective function more than zero is to be chosen as a new QCL structure. Comparing to the initial QCL structure, if the operating wavelength of new QCL structure decreases, then next inner loop ( $n = 2$ ) is carried out. In this step, many QCL structures are created by regularly changing the second pair ( $n = 2$ ) of each quantum well and barrier in active region and the QCL structure is chosen by repetition. After the determination of the fourth well/barrier pair, the thicknesses of the first pair of well and barrier layers are changed again because each layer was correlated with the subband wave functions. So, in the same way, inner loop is infinitely circulated with reiterating from  $n = 1$  to the number of quantum well in active region ( $n = 4$ ). If wavelength no more decreases in spite of change of all pairs of quantum well and barrier in active region, the objective function is saturated and DIF loops finished. The  $k$  represents the convergence counter. If  $k$  is 4 in four quantum well active region, the loop is finished because the wavelength does not more decrease as to previous evaluation for  $k > 4$ . Thus, the last obtained structure of QCL was finally designed QCL structure by the self-consistent numerical technique.

We changed the In mole fraction of  $\text{In}_x\text{Ga}_{1-x}\text{As}$  and  $\text{In}_y\text{Al}_{1-y}\text{As}$

strain-compensated layers from the previously reported QCL operating at  $\lambda \sim 6 \mu\text{m}$  [5] and the self-consistent algorithm was used. Fig. 2 shows the simulation results of  $\text{In}_{0.64}\text{Ga}_{0.36}\text{As}/\text{In}_{0.38}\text{Al}_{0.62}\text{As}$  ( $\Delta E_c = 725 \text{ meV}$ ),  $\text{In}_{0.68}\text{Ga}_{0.32}\text{As}/\text{In}_{0.34}\text{Al}_{0.66}\text{As}$  ( $\Delta E_c = 791 \text{ meV}$ ), and  $\text{In}_{0.72}\text{Ga}_{0.28}\text{As}/\text{In}_{0.3}\text{Al}_{0.7}\text{As}$  ( $\Delta E_c = 876 \text{ meV}$ ) QCL structures. The inset of Fig. 2 shows the conduction band discontinuity as a function of indium mole fraction. The  $\Delta E_c$  is increased to 876 meV (i.e, increase by 73.4 %) for  $\text{In}_{0.72}\text{Ga}_{0.28}\text{As}/\text{In}_{0.3}\text{Al}_{0.7}\text{As}$  compared to the lattice-matched  $\text{In}_{0.52}\text{Al}_{0.48}\text{As}/\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  to InP. This leads to the reduction in leakage current to continuum and the wavelength for light becomes shorter. The wavelengths (objective functions) of saturated QCL structures in each conduction discontinuity are  $2.84 \mu\text{m}$  ( $0.343 \text{ ps}\cdot\text{nm}^2$ ),  $3.125 \mu\text{m}$  ( $0.327 \text{ ps}\cdot\text{nm}^2$ ) and  $3.28 \mu\text{m}$  ( $0.249 \text{ ps}\cdot\text{nm}^2$ ). With larger conduction discontinuity, the emission wavelength could be more shortened by self-consistent design.

Fig. 3 shows the schematic conduction band diagram of a designed  $\text{In}_{0.72}\text{Ga}_{0.28}\text{As}/\text{In}_{0.3}\text{Al}_{0.7}\text{As}$  structure. The emission wavelength is  $\lambda = 2.84 \mu\text{m}$  under applied electric field of 94 kV/cm at 300 K. It has a short lifetime of  $\tau_3 = 0.55 \text{ ps}$  for  $n = 3$  and the electron scattering time from level 4 to level 3 is  $\tau_{43} = 1.21 \text{ ps}$ . The dipole matrix element is  $z_{43} = 0.57 \text{ nm}$ . The designed active region consists of four  $\text{In}_{0.72}\text{Ga}_{0.28}\text{As}/\text{In}_{0.3}\text{Al}_{0.7}\text{As}$  barrier/well pairs: (8.00/0.51), (2.03/2.00), (0.95/4.05), (1.99/3.60) in nm and injector contains six barrier/well pairs: (2.3/3.0), (1.8/2.7), (1.9/2.3), (2.0/2.2), (2.2/2.1), (2.8/2.1) in nm. This designed QCL structure based on a vertical transition which has large optical gain due to the strong spatial overlap between wave functions of the laser transitions compared to the diagonal transition.

In conclusion, we designed the strain-compensated  $\text{In}_{0.72}\text{Ga}_{0.28}\text{As}/\text{In}_{0.3}\text{Al}_{0.7}\text{As}$  QCL structure by using DIF loops algorithm. The shorter wavelength was achieved up to  $\lambda \sim 2.8 \mu\text{m}$  with vertical transition and large conduction band discontinuity ( $\Delta E_c = 876 \text{ meV}$ ) which is increased by 73.4 % compared to the lattice matched structure.

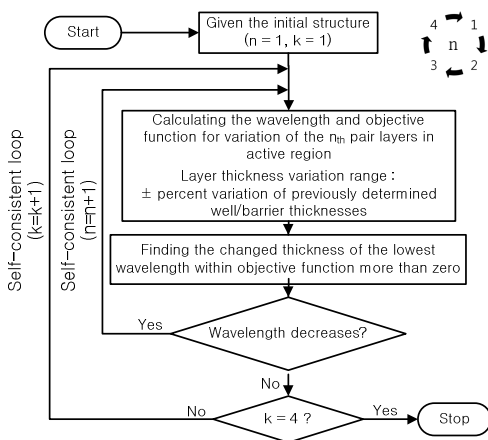


Fig. 1. Self-consistent calculation algorithm of DIF loops.

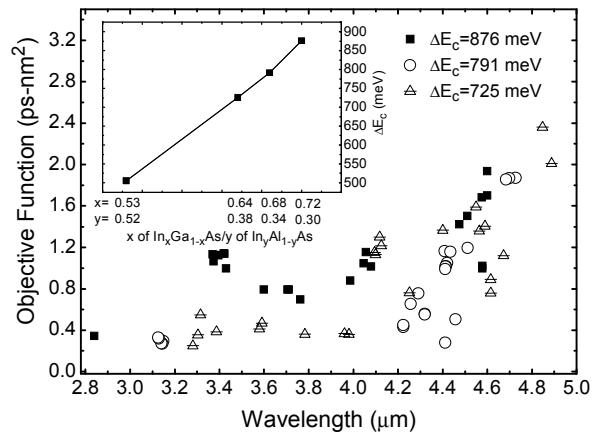


Fig. 2. Simulation results of  $\text{In}_{0.64}\text{Ga}_{0.36}\text{As}/\text{In}_{0.38}\text{Al}_{0.62}\text{As}$  ( $\Delta E_c = 725 \text{ meV}$ ),  $\text{In}_{0.68}\text{Ga}_{0.32}\text{As}/\text{In}_{0.34}\text{Al}_{0.66}\text{As}$  ( $\Delta E_c = 791 \text{ meV}$ ), and  $\text{In}_{0.72}\text{Ga}_{0.28}\text{As}/\text{In}_{0.3}\text{Al}_{0.7}\text{As}$  ( $\Delta E_c = 876 \text{ meV}$ ) QCL structures. The inset shows the conduction band discontinuity as a function of indium mole fraction.

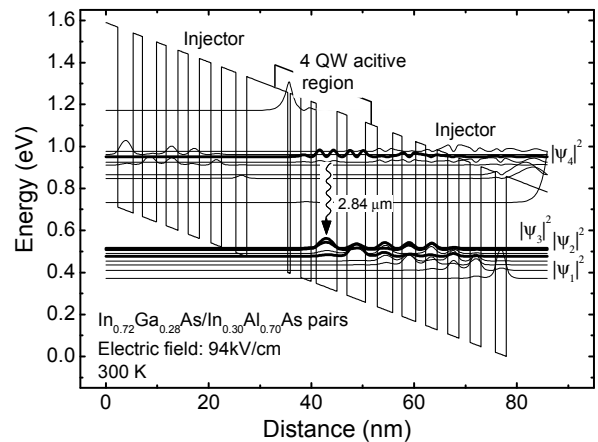


Fig. 3. Schematic conduction band diagram of a designed  $\text{In}_{0.72}\text{Ga}_{0.28}\text{As}/\text{In}_{0.3}\text{Al}_{0.7}\text{As}$  structure.

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