Two-dimensional Simulation of Mid-infrared Quantum Cascade Lasers: Temperature and Field Dependent Analysis

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***Abstract*-We report on a 2D simulation study of a couple of mid-infrared quantum cascade lasers based on the integration of a number of optoelectronic models. Quantum mechanical computation was performed to find the quantization states and a rate equation approach was used to compute the optical gain. Temperature and field dependence effects are taken into account in optical gain model to make a realistic simulation of QCLs. The simulation study compared the integrated models with experimental data with different structures and at different temperatures. Reasonable agreements between experiment and simulation have been obtained.**

I. INTRODUCTION

Quantum cascade lasers (QCLs) can be modeled in various ways, from rate equation model, Monte-Carlo simulations, non-equilibrium Green's function, to density matrix model. Most of these models focus on the carrier dynamics and optical gain in a short range, usually one and a half periods, without a comprehensive simulation of the global devices.We have reported a comprehensive simulation model of QCLs based on integration of a number of optoelectronic models on both microscopic and macroscopic scales[1].On the microscopic scale, quantum mechanical computation was performed to find the quantization states and a rate equation approach was used to compute the optical gain. On the macroscopic scale, we solved transport equations based on nonlocal transport model to account for long-range carrier transport in the device. This model has been implemented in commercial simulation software LASTIP and PICS3D[2].

In our previous articles[3,4], simulation studies of carrier transport properties of mid-infrared QCLs based on non-local transport model have been discussed. In this paper we will focus on a temperature and field dependent analysis of gain model based on simulation of a couple of mid-infrared QCLs with different structures at different temperatures.

II. OPTICAL GAIN MODEL

A critical quantity in QCL modeling is the optical gain which can be expressed as follows for sub-band transition from level j to level i [5]:

$$g = g_0 (n_j - n_i) \tag{1}$$

Here g_0 is the gain coefficient:

$$g_0 = \frac{\pi E |M_{ij}|^2 f_b(E - E_{ij})}{h n_r c_0 \varepsilon_0 t_p} \tag{2}$$

where E is the photon energy, n_r is the real part of the refractive index and t_p is the QCL period thickness. The dipole moment can be written as

$$|M_{ij}|^2 = q^2 |\langle i | z | j \rangle|^2 \tag{3}$$

and the normalized gain spectrum broadening function is given by

$$f_b(E - E_{ij}) = \frac{\tau_g}{h\sqrt{2\pi}} \exp\{-(1/2)[(E - E_{ij})\tau_g / h]^2\} \tag{4}$$

where τ_g is the gain broadening lifetime.

The optical gain described above is sufficient for low temperature and unity injection from injector to active region. Usually there are four major factors which will reduce gain when temperature is high or resonant condition is not satisfied[6]. Firstly,the width of gain spectrum is broadened at higher temperatures. Secondly, electron scattering times for LO phonon emission are reduced by the Bose factor through the larger phonon population at higher temperatures. In addition, extrinsic electrons from the injector region can be thermally excited back into the bottom laser level, where they reduce population inversion. Finally, injection into upper laser level is most efficient at a resonant field and it will reduce when resonant between ground level of injector and upper laser level is not satisfied. To make a realistic simulation of QCLs,temperature and field dependent effects described above should be taken into account, which we will give a detailed discussion in the full paper.

III. RESULTS AND DISCUSSION

The structure studied here is a three-well active region QCL with 75 periods and lasing at 7.8 um based on $In_{0.53}Ga_{0.47}As/Al_{0.48}In_{0.52}As$ multiple quantum wells lattice matched to InP. Specific details and experimental results can be found in [7].

By solving the Schrodinger's and Poisson's equations self-consistently in the microscopic project, one can obtain sub-band diagram as well as the electron wave functions for a QCL. A two-period band diagram and the squared amplitude of the wave functions of the modeled device under resonant field

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of 45 kV/cm are shown in Fig. 1. The levels involved in lasing transition are plotted with red lines. With the sub-band electron distribution obtained from rate equation, all the possible inter-subband transition gains are calculated, as shown in Fig. 2. With the current increasing from 10 to 1000 mA, a strong gain peak at λ=8 μm can be seen, corresponding to energy difference E_{32}=159 meV as shown in Fig. 1.

Multiple lateral optical modes were computed by solving a scalar wave equation as an eigenvalue problem. 2D optical field distribution is shown in Fig.3. Finally, multiple lateral mode laser cavity photon rate equations were solved with the transport equations in a self-consistent manner to predict the lasing characteristics of a quantum cascade laser. Simulated I-L characteristics at different temperatures show reasonable agreement with experimentalresults, as illustrated in Fig.4.

IV. CONCLUSION

We have presented a 2D simulation of a conventional InGaAs/InAlAs QCL, starting from microscopic rate equation to 2D electrical and optical simulations. To verify the efficiency of this model, several other InGaAs/ InAlAs QCLs over different periods at different operating temperatures are also simulated, which will be shown in a full paper in the future.

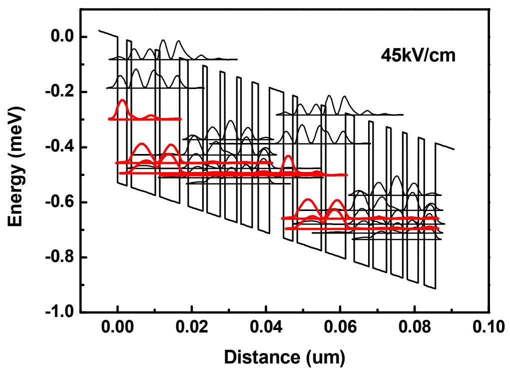

Fig.1 Conduction band diagram and the squared amplitude of the wave functions in two periods of active/injector region at 45 kV/cm; levels involved in lasing transition are plotted with red lines.

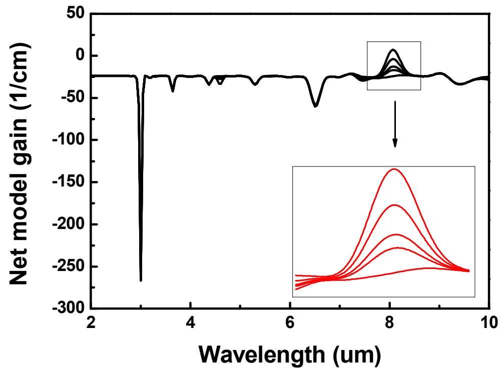

Fig.2 Net modal gain spectra at current ranging from 10 to 1000 mA with an increment of 200 mA. Inset: partial enlarged view of gain peak

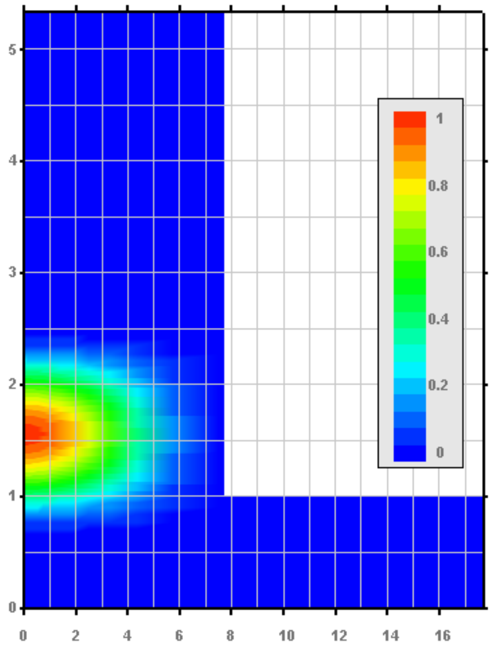

Fig.3 2D optical field distribution of a deep etched ridge waveguide QCL

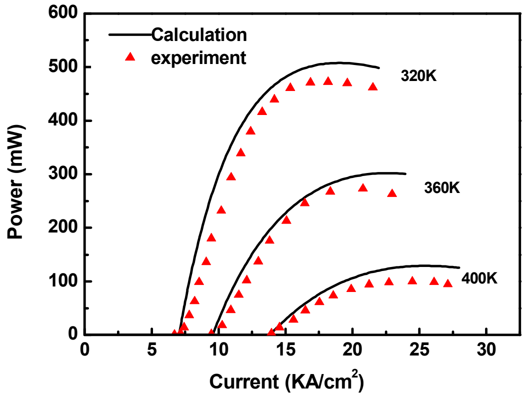

Fig.4 Simulated and experimental J-L characteristics of a 75-period QCLat 320, 360, and 400 K.

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