STSM REPORT

COST STSM Reference Number: COST-STSM-BM1205-32310

STSM Applicant: Aleksandar Demić

STSM Topic: Optical feedback effect and interferometry with quantum cascade lasers

Home Institution: School of Electrical Engineering, University of Belgrade, Belgrade (RS)

Host Institution: School of Electronic and Electrical Engineering, University of Leeds, Leeds (UK)

STSM period: 2016-01-13 00:00:00 to 2016-02-07

COST Action: BM1205

STSM purpose: The goal of this short term scientific mission is for the applicant to gain knowledge in self-mixing interferometry in mid-infrared (MIR) and terahertz (THz) quantum cascade lasers (QCLs), and improve existing model at School of Electronic and Electrical Engineering, University of Leeds, in numerical and theoretical sense. In particular, the theoretical model can provide results which agree very well with experiment, but it is time consuming due to its complexity. Model can be further refined by using parallel computing approaches during the mission.

Description of the main results obtained:

1. Introduction

Bound-to-continuum (BTC) THz QCL structure is commonly used in applications where reasonably low threshold current is needed in order to achieve continuous-wave (CW) operation. BTC QCL has large number of quantum well and barrier layers in one active region period and corresponds to substantial number of quantum-confined subbands involved in electron transport, therefore development of proper theoretical model for electron transport in it is a challenging task.

Model developed in School of Electronic and Electrical Engineering at University of Leeds uses the full rate equation (RE) approach, where all relevant electron states are considered and this is used to derive detailed information about the intersubband transitions, with the dependencies of scattering processes upon lattice temperature and external bias (terminal voltage). Carrier transport model self-consistently solves Schrödinger's and Poisson's equation in conjunction to energy balance equation taking into account interface-roughness, impurity, AC-phonon and LO-phonon scatterings.

In order to theoretically determine I-V behaviour of the design one needs to simulate the structure over the range of external biases and this can be time-consuming due to the large computation time (one simulation of BTC QCL usually lasts for 2 hours). During this STSM existing model was improved in numerical sense and faster extraction of simulation results along with efficient way of displaying output data is now possible.

Self-mixing interferometry needs to take into account the light that returns to the laser cavity after a reflection on the target [1]. This results in terminal voltage oscillations which hold the information of target's properties, thus it is possible to obtain source and the detector within the same device. Physical modelling of this effect can be done by using Lang-Kobayashi optical feedback [2] with reduced rate equation (RRE) approach [3] which is currently being done by the group in Leeds, UK and Brisbane, Australia. RRE approach considers three level system whose parameters are obtained from full RE solution, thus fast extraction of RE results is desired.

2. Numerical challenges and improvements

Since one BTC QCL simulation lasts for 2 hours it is clear that sweeping through moderately sufficient number of external bias points (20-40) can last for couple of days. Fortunately these simulations are independent and it is possible to run each simulation on separate cores of multicore processors. This was done by making use of ARC2 (Advanced Research Computing 2), part of the High Performance Computing facilities at the University of Leeds, which offers over 3000 cores for usage in scientific research at the University.

Initial sweeping script was upgraded with the possibility to spread each simulation point to the cores on the ARC2. By doing this, it is possible to obtain sweep results in time needed for a single simulation (around 2 hours). Script was also upgraded with the possibility to sweep any parameter of QCL (such as lattice temperature, interface roughness parameters etc.) and to allow sweeping through custom defined points (which may be beneficial if we are interested in behaviour around some specific value of external bias).

Additional improvements of the codes were added in terms of plotting, these simulation are performed on Linux operating system, and Grace is commonly used for displaying data (although Gnuplot and Matlab can also be used for data analysis). Grace doesn't allow command line control of plot options, therefor if some result needs to be plotted many times, it can be tiresome to manually adjust visual settings every time. Fortunately Grace allows settings via setup script which is too complicated for the user to understand at the first sight, thus a script which writes setup script for Grace was developed. At this moment it is possible to set plot options via command line, and those options include axis labels, line thicknesses, zooming, grid etc. but also an option for subplots and automatic saving of the graphs.

Script which extracts sweep simulation results is also developed and it also holds a possibility to make a .gif file (by using plot script) out of any single simulation result. This is mostly interesting in terms of wavefunctions and it will be presented in the following section.

3. Numerical results

In this STSM, analysed BTC QCL structure is designed for 2 THz emission and based on design presented in Ref [4]. Fig. 1 shows the band structure diagram, calculated using the full self-consistent Schrödinger–Poisson energy balance scattering transport method [5,6]. Calculations predict emission of 2.06 THz at 20K, see Fig. 2 a), where calculated gain spectra at 20K is presented.

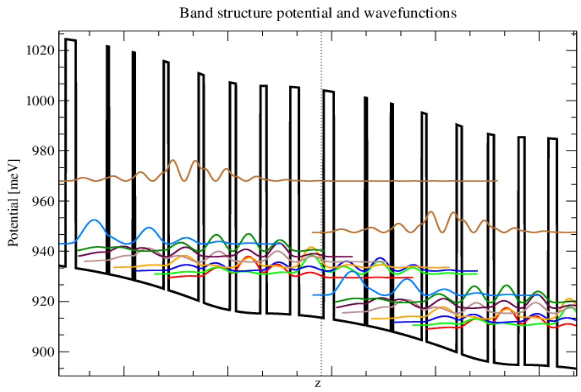

Fig 1. Layer thicknesses for analysing BTC QCL design, starting from the injection barrier (until dotted horizontal line), are **4.8**/15.03/**1.0**/11.54/**0.99**/13.82/**2.3**/14.53/**2.5**/*12.54*/**2.9**/*11.78*/**3.0**/11.4/**4.2**/11.97 $Al_{0.1}Ga_{0.9}As$ barriers are shown in bold and wells doped at 1.3 10^{16} cm^{-3} are underlined. Two periods are presented along with corresponding wavefunctions, applied electric field is 1.65 kV/cm.

Based on the design in Fig 1, L1071_C6_S3 THz QCL wafer was grown via molecular beam epitaxy (MBE) in an Oxford Instruments V-80 H MBE system on a semi-insulating GaAs substrate. The laser material typically consists of 110 repeat periods of $Al_{0.10}Ga_{0.90}As$/GaAs. The ~13.5 µm thick active region is sandwiched between an upper 80 nm thick n+ GaAs layer and a lower 700 nm thick n+ GaAs layer. The latter layer allows the wafer to be processed into single metal QCLs. The wafer was processed into a semi-insulating surface-plasmon ridge waveguide of width 200 µm and cleaved to a length of 3 mm. Thus dimensions of the device are ~14.2 × 200 × 3000 um (height × width × length), these values are used to rescale current density versus electric field from fig 3. into I-V characteristic (Voltage=Electric field * height, Current=Current density * width * length). Such IV curve doesn't have same slope as experimental one due to the neglected contact resistance, in order to fit the curve to the experiment (fig 2b) contact resistance of 2.72 Ω is taken into account.

Device has been characterized in Leeds's Photonic THz Laboratory under liquid He cryogenic conditions. Special attention was paid in analysing fabricated structures that have been theoretically predicted to operate in continuous-wave mode up to 50K operating at around 2 THz. This structure was spectroscopy characterized in pulsed and CW mode up to operation temperature of 55K in pulsed mode (167Hz, 10kHz, 2% duty cycle) and 27K in continuous wave mode. A very good agreement is obtained once (realistic) contact resistance of 2.72 Ω is taken into account in fig 2b. In addition to well documented agreement between measured and calculated *I-V* characteristics, value of driving current when structure starts to abruptly loose optical power, around 1.1 A, agreed well with calculated negative-differential resistivity (NDR) region of around 1.2 A. This behaviour value is caused by theoretically predicted misalignment of subband levels, i.e. reduced electron transports throughout injection barrier.

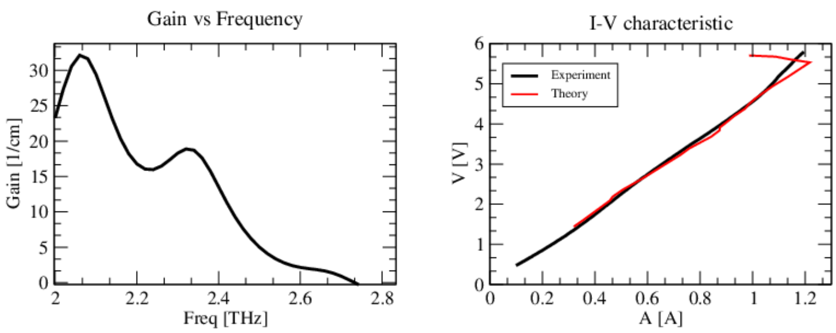

Fig 2. a) Gain versus frequency – The graph shows that lasing emission is expected around 2.06 THz. b) I-V characteristic of the experimental and theoretical data at 20K, contact resistance is 2.72 Ω.

Current-voltage (I-V) characteristic of the device can be calculated by sweeping applied electric field (terminal voltage) assuming homogeny distribution of electric field across the heterostructure. In the first instance, calculated I-V characteristics of QCL device assumes that total terminal voltage is distributed across the active region i.e. voltage drops on the contacts is neglected. In order to fit theoretical data to the experiment, including non-zero contact resistance would be needed in the model as it was done in fig. 2.

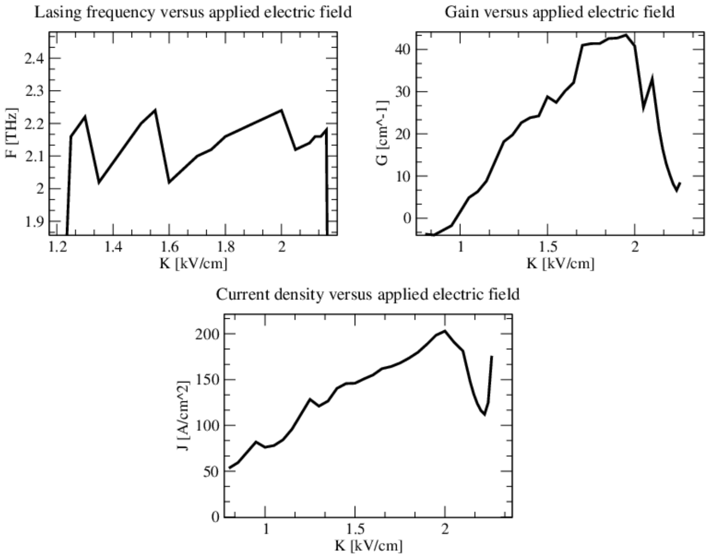

Fig 3. Frequency, gain, and current density versus applied electric field.

In fig. 2a Gain versus frequency for fixed value of bias is presented, if coordinates of the maximum point in fig. 2a are extracted for each sweep point, it is possible to obtain first two graphs on fig. 3. Lasing will occur on bias point whose gain overcomes cavity losses, in this structure losses are assumed to be 30 cm^{-1}, this is obtained for electric field of 1.65 kV/cm, and results in lasing emission of 2.06 THz.

In RE approach Current density (and Gain) exhibits formation of unrealistic spikes which are usually omitted in final results because these situations correspond to non-physical behaviour of the device. On fig. 3 only couple of these spikes occur. Formation of these spikes comes from the fact that coherent transport is not taken into account with RE approach, thus it is possible for two states to have very pronounced optical transition which ignores the existence of tunnelling through a barrier of finite width, naturally this results in unrealistic values of current density and optical gain.

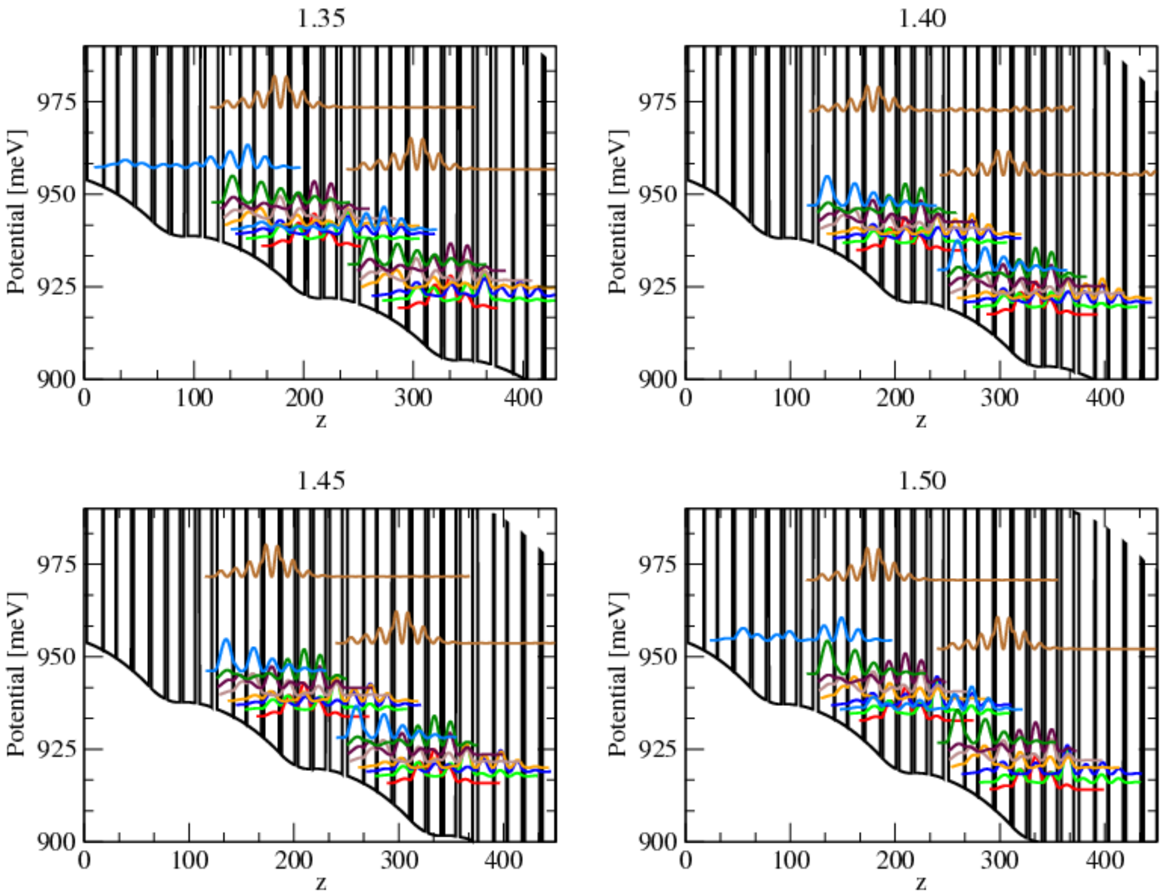

Fig 4. Two period potential and corresponding wavefunctions for a) 1.35 kV/cm b) 1.40 kV/cm c) 1.45 kV/cm d) 1.50 kV/cm

In fig. 4 wavefunctions in two periods are presented. Every time hybridization of the states from two periods is about to occur, non-physical behaviour happens and results in a spike in current density. Around 1.4 kV/cm such spike occurred and on fig.4 we can see that prior to hybridazation (for 1.35 kV/cm) 9^{th} state from second period nearly matched 8^{th} state from the first period. For the 1.4 kV/cm and 1.45 kV/cm hybridization occurred and this resulted in spike in fig. 3. These non – physical points are even more noticable when smaller electric field step is chosen in the simulation (because lining of states from different periods is more probable). In fig 3. step of 0.05 kV/cm was chosen in a way that the spikes are barely noticable.

4. Mutual benefits for the Home and Host institutions

Collaboration with the host, Dr Dragan Indjin from the School of Electronic and Electrical Engineering, University of Leeds, was very useful and stimulating, existing RE model was numerically upgraded and now allows fast extraction of the results. Both groups have a better understanding of possible critical areas in the simulation which require further work specially for further development of self-mixing interferometry models.

Acknowledgment

I would like to express gratitude to Dr Alexander Valavanis and Dr Andrew Greer on explanations and discussions regarding QCL simulation codes which are being developed at School of Electronic and Electrical Engineering, University of Leeds. My sincere thanks also go to Ms Reshma Anamari Mohandas and Dr Alexander Valavanis for experimental support and results for 2THz BTC-QCL and finally I'd like to thank the host Dr Dragan Indjin on his support, discussions and guidance during the visit.

References

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STSM outcome form

STSM application number	Home institution & country	Host institution & country	BM1205 WG	Objective of the collaboration	Results of the collaboration
COST-STSM-BM1205-32310	School of Electrical Engineering, University of Belgrade, Serbia	School of Electronic and Electrical Engineering, University of Leeds, UK	WG2/WG3	Self-mixing interferometry understanding and optimizing numerical results from existing (non feedback) model	- parallelization of the initial simulation code - development of the code which automatically extracts the results with the possibility of .gif making - development of automatic plotting code -Simulation of the BTC 2THz QCL and comparison with experimental results

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Confirmation of successful execution of the STSM

To the Grant Holder of the COST Action BM1205

STSM Participant: Aleksandar Demić

Home Institution: School of Electrical Engineering, University of Belgrade, Serbia

Host Institution: School of Electronic and electrical Engineering, University of Leeds, UK

I hereby confirm the successful completion of the STSM entitled "Optical feedback effect and interferometry with quantum cascade lasers" carried out by Mr. Aleksandar Demić, at the Institute of Microwaves and Photonics, School of Electronic and Electrical Engineering, University of Leeds in the period 13/01/2016 to 07/02/2016.

The STSM was completed according to the work plan described by Mr Aleksandar Demić in the STSM.
Application and the most important results are presented in his report. The STSM had a mutual benefit for the applicant and the host group, in consideration of both the particular research activities that were performed and the expected strengthening of cooperation between the applicant's and the Host institution.

Yours sincerely,

First name and last name: Dragan Indjin,

Dragan Indjin

Signature: ________________