STSM report

STSM Application number:
010515-058490

STSM Grantee:
Andrew Grier

STSM title:
Development and comparison of simulation tools for THz QCLs

Home Institution:
University of Leeds, Leeds, United Kingdom

Host Institution:
Lund University, Lund, Sweden

STSM period:
12–19 May 2015

STSM purpose:
Comparative modelling of THz QCLs to develop predictive tools in laser design

Description of the work carried out during the STSM:

Quantum cascade lasers are compact, coherent sources of THz radiation which have many practical applications ranging from medical to security screening. Advances in understanding of device physics by intensive theoretical research have contributed to the peak operating temperature increasing to 200 K in 2012 [1]. Predictive models allow the use of optimisation techniques such as genetic or simulated annealing algorithms. Some success has already been reported with this approach [2], however an improvement on the highest operating temperature remains elusive. Additionally, the development of models which include the effect of self mixing interferometry require the ability to capture free-running laser characteristics as an initial starting point.

Several significantly different modelling approaches with increasing levels of complexity exist: rate equations, density matrices, and non-equilibrium Green's functions. The latter two approaches are those used at Leeds and Lund Universities respectively, and the DM approach is significantly less computationally demanding. To be used as design/optimiser tools they are required to accurately replicate experimentally results. However, since experimental measurements have unpredictable problems such as contact resistances, contact drops, and defects, this is often hard to test. In this mission we compare the DM and NEGF model with synchronised material parameters, interface roughness estimates and temperatures to test a) what experimental features cannot be explained theoretically and b) whether the DM approach is capable of capturing the necessary physics to be used as a successful design optimiser and/or an approach which a self mixing model can be built on to.

As the objective of the work is accurate modeling of high temperature operation, and operation of devices used for interferometric applications, the models were applied to the current 200 K reference structure [1] and a higher doped version of the bound to continuum (BTC) structure in Ref [3]. In the bound to continuum structure case, the active region depends on transport between 9 confined states, rather than the 4 typically relevant in resonant phonon structures. Therefore modelling is expected to be significantly more complex due to the additional time necessary to do calculations. Additionally, it was expected that such complicated structures would reveal inadequecies and weaknesses of each model. Details of the NEGF and DM models can be found in Refs. [4] and [5] respectively.

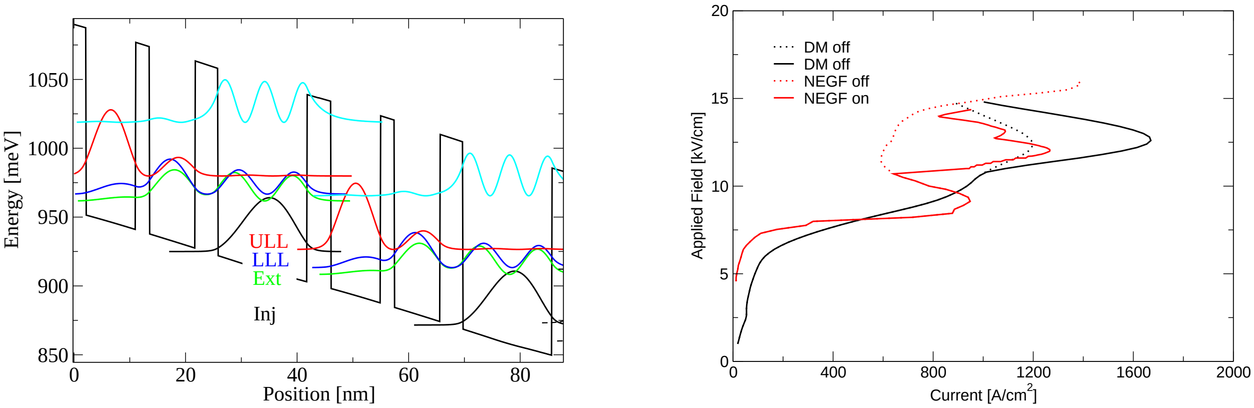

Figure 1: Left: Bandstructure and wavefunction plot for the 200 K reference structure at 12.2 kV/cm. Right: I–V characteristics calculated with both DM and NEGF models for a lattice temperature of 50 K.

Description of the main results obtained:

The states used for the calculation of the current record holder is shown in Fig. 1(a) at its design bias of 12.2 kV/cm. Fig. 1(b) shows the calculated I–V characteristics of the investigated structure using both NEGF and DM models. Both models correctly predict the lasing threshold voltage, indicating good agreement of the state engergies and bandstructure parameters. The raw experimental data for the current world record structure was not available, however both compare well with the results presented in Fig. 3 in Ref. [1].

Some disagreement between the models can be observed; the main difference being the NDR predicted by the NEGF model during laser operation. The cause of this is the shift in energy levels caused by fast scattering as states become aligned. It is noted that the magnitude of the photon driven current caused by the device lasing are in good agreement with each other and with experiment. This indicates both that light interaction is handled correctly in the model, and that the choice of 20 cm^{-1} for the waveguide losses is a good estimate.

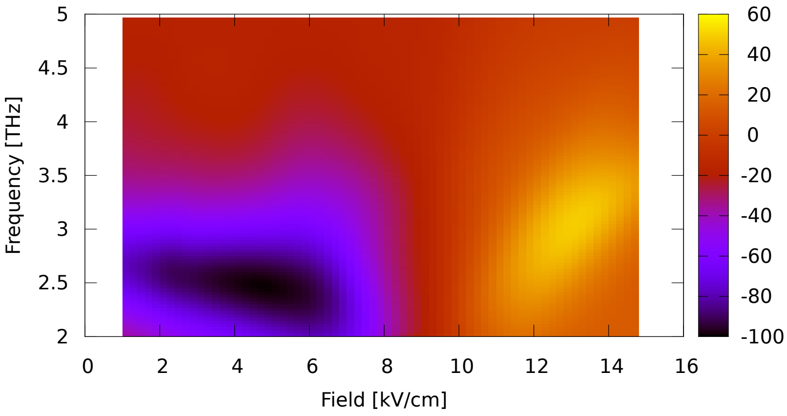

Figure 2: Unsaturated gain (per cm) versus applied field and Frequency for the reference structure. The peak gain offered agrees well with the experimentally observed lasing frequency of 2.8–3.2THz at different temperatures and driving currents shown in Ref [1]

Fig. 2 shows the gain for the reference structure at 50 K versus both applied field and frequency. This plot shows the shift in peak gain available for the laser shift from 2.8 THz to 3.2 THz as the applied field shifts from 11.0 kV/cm to the design bias of 12.2 kV/cm. This agrees well with the experimentally observed frequencies shown in Ref. [1]. For this structure we conclude that the DM model includes sufficient detail of the QCL transport to be a good predictor and allow its use as a design tool.

The BTC structure is significantly more complex since a significant number more quantum states need to be accounted for. Since matrix based calculations (of which both DM and NEGF models are) typically increase in time taken with N^2, where N is the number of states per period, the increase from 4 states for the 200 K reference structure to the 9 in the BTC structure is potentially computationally expensive. We note that no previous studies of BTC THz QCLs are available in the current literature, and that the application of our model to these structures is suitably novel for publication. Fig 3 shows the states and bandstructure of the device illustrating the importance of the inclusion of the Poisson field caused by the distribution of the electrons. Population inversion in this structure is achieved by the miniband of overlapping states below the LLL rather than a fast extraction by LO phonons used in the high-temperature structures.

Fig 3(b) shows the model results for the BTC QCL along with the experimental data of a device grown at Leeds (shared by P. Dean and J. Keeley at the University of Leeds). Good agreement with the experimental peak current density is observed for the DM model however the NEGF model overestimates this. This is attributed to the difficulty in modelling the fast intrasubband scattering needed to thermalise the subband in the NEGF model, while the DM model avoids this problem by assuming some fixed electron temperature for all subbands. It is shown that there is a significant difference in the voltage position of the peak current. Since this is present for both models, we can then assign this to experimental characteristics of the device i.e. a voltage drop or a series resistance.

Voltage drops that cause an offset between theoretical and experimental current characteristics can be caused by Schotty contacts as metal waveguides/contacts are deposited on the semiconductor GaAs. These contribute some fixed voltage in addition to the potential across the device active region. In addition to this, the contacts and experimental bonds will add a resistance value which has an increasing voltage shift with increasing current. The 200 K record structure shown in Ref. [1] has different voltage shifts for different waveguide materials, however we chose to compare with a growth of the same structure reported in Ref. [6]. This has similar performance to the record structure but has a clearer presence of contact resistance. Comparisons for both reference and BTC structures are made in 4 with the model now accounting for these effects. Contact resistances of approximately 1Ω were used, and in the case of the reference structure in Ref. [6], a voltage drop of 5 V was used to obtain agreement.

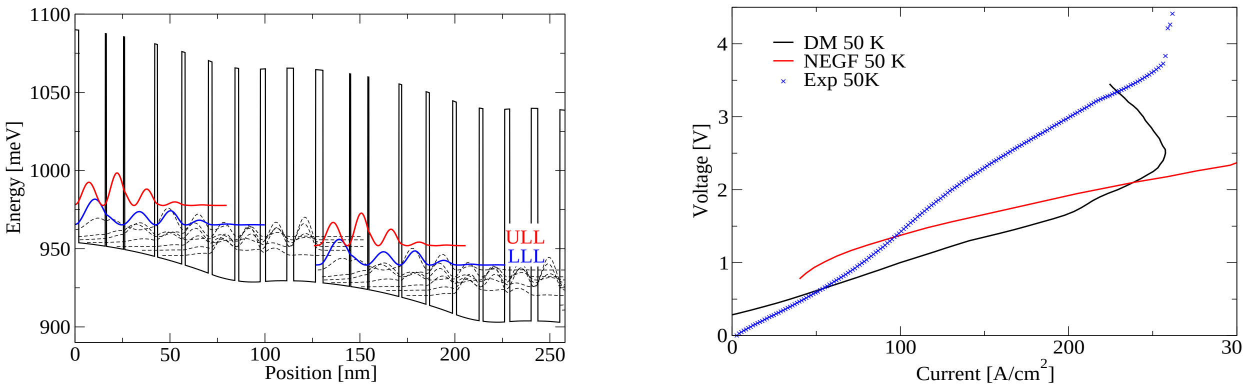

Figure 3: Left: Bandstructure and wavefunction plot for the BTC device at 2.0 kV/cm. Right: DM and NEGF model results compared with experimental data shared by P. Dean and J. Keeley at the University of Leeds.

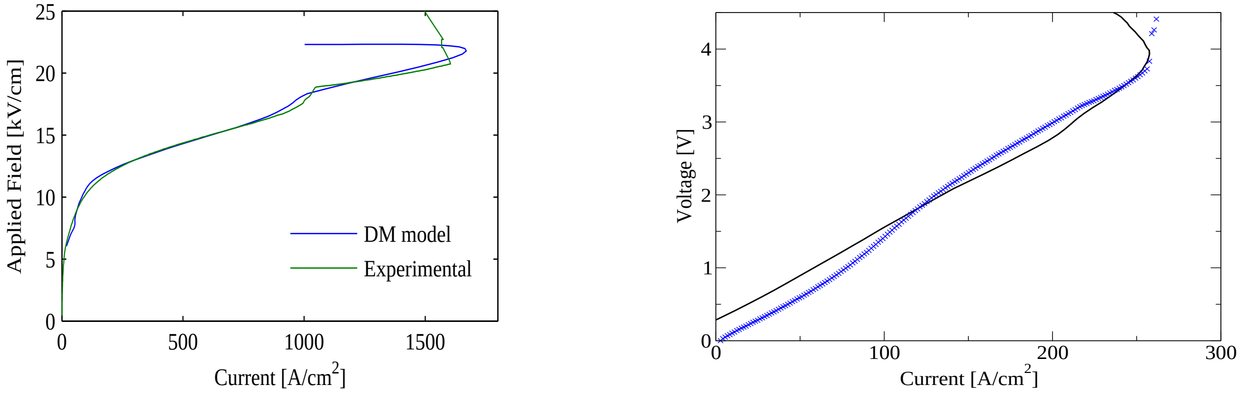

Figure 4: Left: DM results with a voltage drop of 5 V and a contact resistance of ≈1Ω applied. Experimental data from Ref. [6] kindly shared by I. W. Chan at MIT.
Right: Applying contact resistance to the DM model output (green) line improves agreement with experimental data (blue crosses)

Mutual benefits for the Home and Host institutions:

This STSM was useful for both groups at the University of Leeds and University of Lund as it enabled the discussion and comparison of significantly different modelling approaches. The University of Leeds has been able to validate its model results by obtaining excellent agreement with both NEGF and experimental data. Researchers were able to discuss the exact methods of calculating the current through these complex devices, which could lead to further refinement of the model.

Future collaboration with the Host institution (if applicable):

As we have successfully demonstrated the applicability of the DM approach in THz QCLs we can now report the results of this comparative work in a journal application. This work has also confirmed that suitability of our DM model for its use as a fast design tool. We intend to apply this to the design of high power and high temperature operation QCLs. This STSM has set the ground work for NEGF modelling to check structures before expensive growth of experimental structures.

Foreseen journal publications or conference presentations expected to result from the STSM (if applicable):

We are confident that the result obtained so far are suitable for publication and will be of interest to the modelling community. A journal article is expected in Q3 2015.

Acknowledgements

The author would like to thank P. Dean and J. Keeley for sharing experimental I–V data for the BTC structure and the associated growth team led by L. Li. and E. H. Linfield. Thanks are also due to I. W. Chan and his colleagues for sharing experimental data for the 200 K structure.

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
STSM-BM1205-010515-058490	University of Leeds, United Kingdom	University of Lund, Sweden	WG 2, WG 3	Development and comparison of simulation tools for THz QCLs	Comparative modelling and validation of models. Models applied to structures suitable for interferometric uses

I confirm that Mr Andrew Grier attended the University of Lund, Sweden and completed an STSM from 12th-19th May 2015.

Signed:

Professor Andreas Wacker

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University of Lund,
Sweden