STSM outcome form

STSM application number	Home institution & country	Host institution & country	BM1205 WG	Objective of the collaboration	Results of the collaboration
STSM-BM1205-180115-054381	University of Lund, Sweden	University of Leeds, United Kingdom	WG 2, 3	Determine capabilities of different QCL models and produce predictive tools in laser design	Several projects in key areas was started. Possible ways of model improvement was found for both parties

I hereby confirm the successful completing of the planned short term scientific mission by David Winge. In addition to giving a seminar during his visit, David and our own research group members discussed in detail the comparative modelling of different quantum cascade laser structures of interest. This was useful for both research groups and plans for further cooperation between Lund and Leeds have been made.

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STSM report

STSM Application number:
STSM-BM1205-180115-054381

STSM Grantee:
David Winge

STSM title:
Comparison of quantum transport simulators to produce predictive tools in laser design

Home Institution:
Lund University, Lund, Sweden

Host Institution:
University of Leeds, Leeds, United Kingdom

STSM period:
17–24 January 2015

STSM purpose:
Collaborative effort to determine capabilities of different QCL models and produce predictive tools in laser design

Description of the work carried out during the STSM:

Thanks to a decade of intensive research into THz quantum cascade laser designs the maximum operating temperature reached $\tilde{2}00$ K in 2012 however further progress has not been reported. Predictive theoretical models offer the possibility of structure optimization and engineering novel designs capable of operation at higher temperature. During this STSM, the main focus is to investigate the bound to continuum (BTC) structure originally realized by Barbieri *et al.* [1] in 2004 since it is currently used for most imaging experiments due to its stable continuous wave (CW) operation.

A main focus of this mission is the different dephasing rates in this structure; these rates will determine the balance in the structure towards coherent and non-coherent transport. A comparative study with both models will give a possibility to address the question whether the transport is mainly coherent or not. The broadening of the states together with correlation effects will determine the linewidth of the gain peak, or if you will, the dynamic range of the gain medium. This is very interesting to look at since it will determine the tenability of the design in frequency space.

Being a report on the advances during the Short Term Scientific Mission, this document is not the correct place for a thorough description of both models used in this comparative study. We will instead use this section to highlight the main differences that are important to consider when analyzing the results below. In addition, we will provide the references needed for the reader to familiarize her or himself in detail with both models.

The model used in Leeds is based on the work previously presented by Dinh *et al.* in Ref. [2]. It is a density matrix (DM) model which uses coherent transport to simulate the transport over the main injection barrier. The system is divided in periods, where the states confined in each period are calculated using a tight-binding Hamiltonian (TODO: Ask Andreas for name) and then coupled across the injection barrier to all other states in the next as well as the previous period. To summarize, the transport between periods is considered coherent whereas intrinsic transport mechanisms, inside each period, are considered incoherent processes. This is an approach that is widely used [3, 4] as it provides results which can be fitted to most experiments. In most implementations, the scattering rates are calculated using Fermi-Dirac statistics using a single effective electron temperature for all subbands.

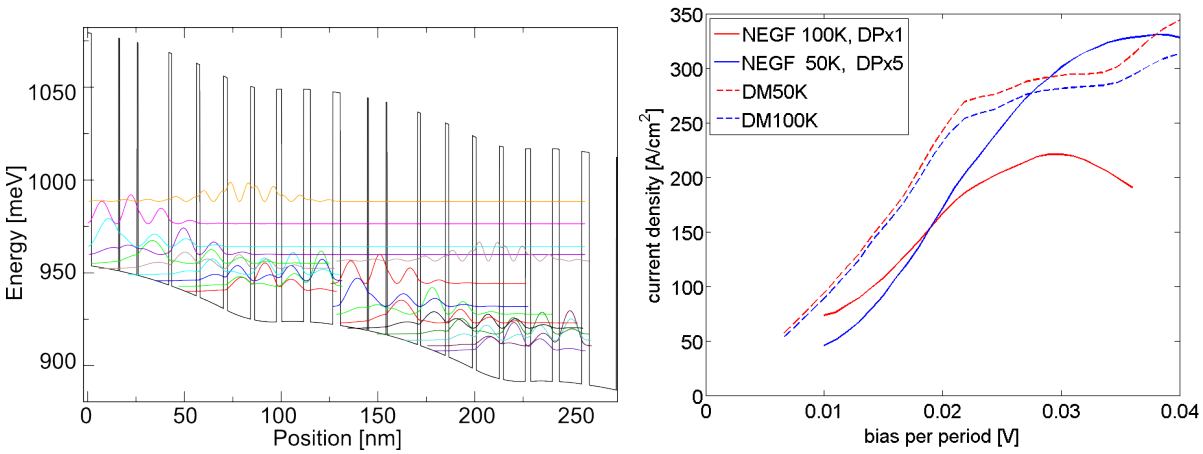

Figure 1: Left: Plotted probability densities for the states confined in the growth direction z plotted at their respective energies. The states are the converged ones from a self-consistent Shrödinger Poisson solver. Right: Comparisons between the models where the current-voltage characteristics have been plotted.

In Lund a model based on non-equilibrium Green's functions is used [5]. Compared to DM models, the formalism allows for the resolution of both states and coherences in energy. In DM models an effective energy has to be used to estimate the energy of a coherence, but in NEGF formalism this is provides by the energy resolved Green's functions. The energy in these objects comes from the fact that correlations of excitations between two different times are considered, which effectively gives the model a concept of memory which then can be used to calculate lifetimes and thus broadening of both states and coherences. Tunneling, i.e. coherent transport, is here allowed between all states and not only across the injection barrier. The populations are calculated self-consistently which means that an effective temperature is not needed but it can be extracted from the simulations. The width of the gain peak is an important parameter that can be hard to model in systems out of equilibrium. As the gain is proportional to the inversion and inversely proportional to the linewidth, it is a dominant factor in determining the temperature range of an operating laser. The main contributions to linewidth are the lifetimes of the upper and lower laser state, but it is also important to consider the correlation between the states. If the electrons in the upper and lower laser state are correlated with respect to the scattering environment, this effect will sharpen the gain transition [6]. Linewidth calculations in the NEGF formalism can this be used to motivate narrowing of gain spectra in the DM model.

Following the outlines in the work plan, the BTC structure was analyzed in great detail using both approaches. This led, among other things, to interesting comparisons of the general electron temperatures used in the Density Matrix (DM) calculations to the self consistently evaluated ones using the non-equilibrium Green's function formalism. Another interesting point of comparison was the width of the gain peak, where the the models produced transferable results.

As the BTC structure is a complex structure with many states per period, simulations were also carried out on a four-well QCL presented in [7]. These structures are based on a resonant optical phonon extraction but have a number of states capable of acting as lower laser states, why they are often called *hybrid designs*. Additionally, the record breaking structure of Fathololoumi *et al.* [8] and a scattering assisted structure [9] which are well studied by theoretical models were compared to validate the models however, these results are not included here.

Description of the main results obtained:

The BTC design is plotted with the states extracted from the DM calculation in Fig. 1. When compared, the two models produces a similar band structure but with obvious differences at the injection barrier due to the tight-binding approach of the DM. Simulations of this structure had already successfully been performed

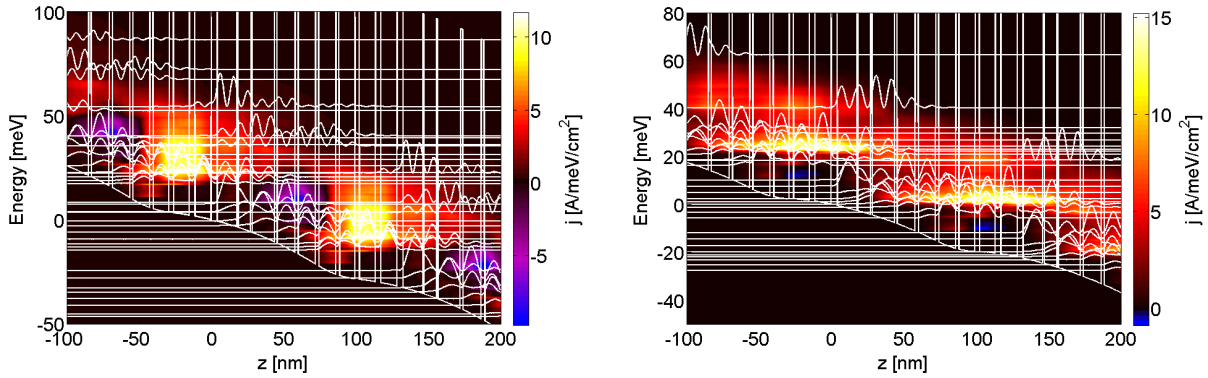

Figure 2: Plots of currents resolved in energy for the case of normal deformation potential (left) and with deformation potential artificially increased to five times its value (right, DP×5).

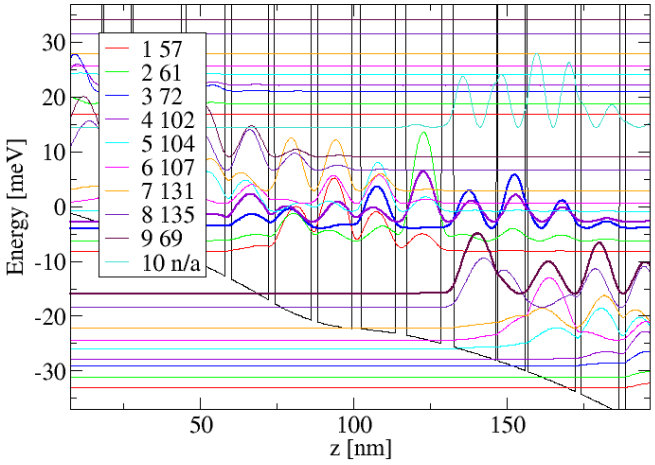

Figure 3: States plotted with their respective electron temperature extracted from the NEGF model.

in Leeds using the DM model. With the NEGF model however, several problems quickly emerged which can tell us a lot about the differences in the models. First of all, convergence was impossible to reach at low temperature. In this report low temperature is defined as a lattice temperature of 50 K. At higher temperatures convergence could be reached, as seen in Fig. 1, although the current is less than the DM equivalent. When examining the current densities resolved in energy at this temperature, displayed in Fig. 2 one can observe that current is not very well conserved over the range of one period. The current should be constant at each point along z which is not the case. This structure highlights one important aspect of the NEGF model. As the electron distributions are calculated from scratch, it is very important to have all scattering mechanism properly accounted for. As carrier-carrier scattering only is implemented at the level of a meanfield potential in the NEGF model, it seems that there is not enough incoherent transport effects in the miniband designed to move electrons from the lower laser state to the next period. In an attempt to compensate for the missing scattering, acoustic phonon scattering was artificially increased. This can then serve as a test to whether more scattering would improve the simulation results. These simulations actually converged better, and the new energy resolved current plotted in Fig. 2 conserves current to a satisfactory degree. These results was also used to establish the principle of comparing the electron subband temperatures. For each subband the non-equilibrium distribution was extracted and fitted to a Fermi-function. This gave

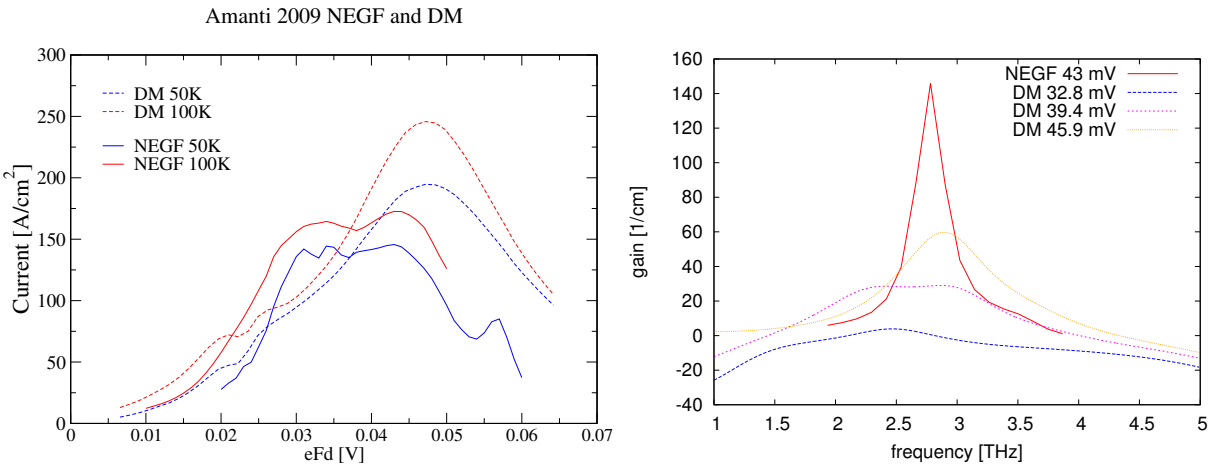

Figure 4: Left: Comparison of the current-field characteristics produced by both models at temperatures of 50 K and 100 K. Right: Comparison of gain calculations with the two models at 50 K lattice temperature.

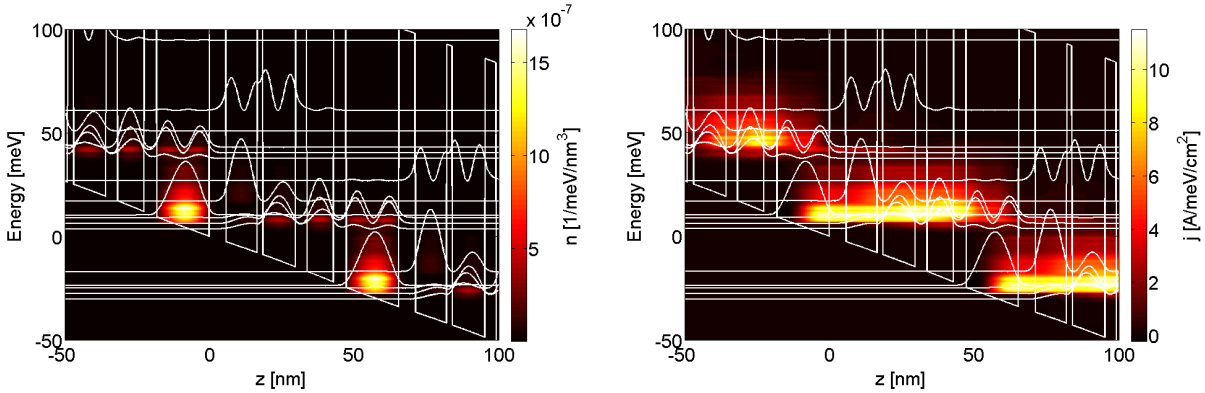

Figure 5: Shown here are energy resolved densities as well as current at the top of the prepeak seen at 34 mV for the NEGF simulations in Fig. 4. Current is made up by coherent tunneling over three barriers.

an effective electron temperature which is showed in the band structure plotted in Fig. 3. At a lattice temperature of 50 K, one observes a ground state (labeled 1) almost thermalized with respect to the lattice while the upper laser state is at a temperature around 50 K higher. This can be compared to the effective temperature used in the DM simulations which in this case was found to be 60.5 K.

The Amanti's 2009 design [7] is a four-well QCL that has received some attention due to its broadband features. It was recently grown in three different versions as a multistack QCL where the emission frequencies of the design had been shifted by moving the barrier next to the injector barrier downstream in the design [10, 11]. It is an interesting structure to compare models on, as it contains both a strong longitudinal phonon extraction and a small band of lower laser states that is typical in BTC designs. Simulation results from both the DM model as well as the NEGF model are compared in Fig. 4. In the left part, current is displayed at two different lattice temperature. The peaks in current are of similar values, although the DM model produces a bit more current. Another feature clearly noticeable is the double peak feature in the NEGF simulations. This is again attributed to the difficulties in the treatment of the scattering mechanisms of the miniband. The right part of Fig. 4 shows a comparison of gain at 50 K lattice temperature. Here we observe a narrow linewidth for the NEGF results while the gain calculated from the DM model at different bias points shows a larger width. This is, among other things, an effect of the correlated electrons in the upper and lower laser state.

In order to investigate the behavior of the NEGF simulations at the first of the two current peak, densities and current are plotted in Fig. 5. Here it is displayed how current via tunneling over at least three

barriers is transported to the first excited state of the widest well. This way an effective transport channel is established, and this has indeed been observed in laser designs with fewer wells [12] but not in these four-well QCLs. The density matrix simulations do not shown the same response at similar biases, but only small alignment features that indicate some long range tunneling. There is a lot to learn here from further collaboration that might benefit the development of both models.

Mutual benefits for the Home and Host institutions:

Collaboration with the University of Leeds was useful, with many aspects of QCL modelling discussed between the grantee and host. By discussing challenges encountered and subsequent work, both groups have a better understanding of possible methods of improvement. The group in Leeds will benefit from the discussion of the NEGF approach for QCL modelling which has several advantages over the density matrix approach.

Future collaboration with the Host instituion:

As stated previously, each model has its own advantages and disadvantages. The DM solver is quick and suitable for design optimizations as it can scan a large part of the parameter space and thus investigate many possible design alternatives [13]. It is made quick by a number of clever approximations that to large extent reproduces the behavior in known experiments. The NEGF model is built in order to model the transport in QCLs from an ab initio perspective, and large effort is put into establishing a basis independent framework which should give the same result no matter the specific implementation of a structure (which is arbitrary since the QCL is periodic) or the kind of basis states used. The resolution of states and coherences in energy is another complication that renders the calculations orders of magnitude slower than the DM equivalents.

One possible area of further collaboration could be the optimization of structures. Here one could imagine quick optimization using the DM solver where different successful outcomes are then analyzed by the NEGF model. There is also a lot to gain from further comparisons of gain width and temperature calculations with experimental data to validate the approaches of both models.

Foreseen journal publications or conference presentations expected to result from the STSM:

We anticipate that the results of this STSM will be used in a forthcoming journal paper. Additionally, we note that there is little published work on simulations of the BTC designs that go beyond rate equation modeling. If the collaboration continues to be fruitful, there can be many interesting results worth publishing.

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