Data information

This repository contains all data that corresponds to figures associated with our publication *“Effects of background doping, interdiffusion and layer thickness fluctuation on the transport characteristics of THz quantum cascade lasers”*.

We have used Grace under Linux platform for generating figures in this work.

Grace is a free WYSIWYG 2D graph plotting tool, for Unix-like operating systems. You can find more info on [https://en.wikipedia.org/wiki/Grace\_(plotting\_tool)](https://en.wikipedia.org/wiki/Grace_%28plotting_tool%29). Grace also has open source support for Windows operating system <https://sourceforge.net/projects/qtgrace/> which uses .agr extension.

To execute .agr file, you simply need to run this command on any Unix-like operating system:

***xmgrace file.agr***

or open the .***agr*** file with qtgrace’s GUI (executable in the link <https://sourceforge.net/projects/qtgrace/> is located in bin/ directory, and no package installation is required).

As with many plotting tools, the data associated with the figures is directly available in the .agr files.

.agr file is an ordinary text file and it can be open with any text editor. We advise Notepad++. Typically, the first set of lines have a form:

# Grace project file

#

@version 50123

@page size 792, 612

@page scroll 5%

@page inout 5%

@link page off

@map font 0 to "Times-Roman", "Times-Roman"

@map font 1 to "Times-Italic", "Times-Italic"

@map font 2 to "Times-Bold", "Times-Bold"

@map font 3 to "Times-BoldItalic", "Times-BoldItalic"

@map font 4 to "Helvetica", "Helvetica"

@map font 5 to "Helvetica-Oblique", "Helvetica-Oblique"

@map font 6 to "Helvetica-Bold", "Helvetica-Bold"

@map font 7 to "Helvetica-BoldOblique", "Helvetica-BoldOblique"

@map font 8 to "Courier", "Courier"

@map font 9 to "Courier-Oblique", "Courier-Oblique"

@map font 10 to "Courier-Bold", "Courier-Bold"

@map font 11 to "Courier-BoldOblique", "Courier-BoldOblique"

@map font 12 to "Symbol", "Symbol"

Lines starting with “@” are instructions for Grace plotting tool. The lines can be easily understood as simple figure settings, they set up x-y limits, colors, legends etc. What is important to understand in this file is how data information is stored.

Every graph in a figure has a label G0, G1, G2 … etc, every trace on a given graph has a label S0, S1, S2 … etc. For a standard x-y plot, only 1 graph and 1 trace exist, and info is stored after the line starting as @target G0.S0, if the plot has multiple traces, next one will be at @target G0.S1 etc.

If the figure has insets or another y-axis. the first graph and its traces would be labeled as G0.S0, G0.S1, G0.S2 … etc, and the inset data would be targeted as G1.S0, G1.S1, G1.S2 … etc.

We decided not to provided data traces directly, as they can be easily found in .agr files after searching @target GX.SY and understanding which trace in the figure corresponds to which target. Additionally, all our graphs can be recreated by simply using . agr file with Grace in Linux or qtgrace in Windows.

The following table lists all . agr figures in our paper and the corresponding GX.SY mapping of the traces represented in them.

|  |  |  |  |
| --- | --- | --- | --- |
| Filename | Graph | Trace | Description |
| Fig1a\_BTC\_background\_doping.agr | G0 (top) | S0 | Material gain $g$ versus external bias $K$ for BTC QCL without background doping |
| S1-S3 | Material gain $g$ versus external bias $K$ for BTC QCL with $n$ background doping concentrations $n\_{B}=1⋅10^{14} cm^{-3}, 5⋅10^{14} cm^{-3}$ and $1⋅10^{15} cm^{-3}$, respectively |
| S4-S6 | Material gain $g$ versus external bias $K$ for BTC QCL with $p$ background doping concentrations $p\_{B}=1⋅10^{14} cm^{-3}, 5⋅10^{14} cm^{-3}$ and $1⋅10^{15} cm^{-3}$, respectively |
| G1 (bottom) | S0 | Current density $J$ versus external bias $K$ for BTC QCL without background doping |
| S1-S3 | Current density $J$ versus external bias $K$ for BTC QCL with $n$ background doping concentrations $n\_{B}=1⋅10^{14} cm^{-3}, 5⋅10^{14} cm^{-3}$ and $1⋅10^{15} cm^{-3}$, respectively |
| S4-S6 | Current density $J$ versus external bias $K$ for BTC QCL with $p$ background doping concentrations $p\_{B}=1⋅10^{14} cm^{-3}, 5⋅10^{14} cm^{-3}$ and $1⋅10^{15} cm^{-3}$, respectively |
| Fig1b\_n\_doping.agr | G0 (top) | S0,S1,S2 | Material gain versus $n$ background doping concentration for LO-phonon, BTC and Hybrid QCL design respectively |
| G1 (middle) | S0,S1,S2 | Current density versus $n$ background doping concentration for LO-phonon, BTC and Hybrid QCL design respectively |
| G2 (bottom) | S0,S1,S2 | Emission frequency versus $n$ background doping concentration for LO-phonon, BTC and Hybrid QCL design respectively |
| Fig1c\_p\_doping.agr | G0 (top) | S0,S1,S2 | Material gain versus $n$ background doping concentration for LO-phonon, BTC and Hybrid QCL design respectively |
| G1 (middle) | S0,S1,S2 | Current density versus $n$ background doping concentration for LO-phonon, BTC and Hybrid QCL design respectively |
| G2 (bottom) | S0,S1,S2 | Emission frequency versus $n$ background doping concentration for LO-phonon, BTC and Hybrid QCL design respectively |
| Fig2a\_Cond\_band\_diffusion\_200K\_LO\_phonon\_potential.agr | G0 | S0, S7, S8 | Bottom of the conduction band potential of the 200 K LO-phonon THz QCL for interdiffusion diffusion lengths $L\_{D}=0, 1.5A, and 3A$  |
| S1-S6 | Wavefunctions squared, 6 states, plotted in light blue |
| Fig2b\_Compositional\_Diffusion.agr | G0 (top) | S0,S1,S2 | Material gain versus interdiffusion diffusion length for LO-phonon, BTC and Hybrid QCL design respectively |
| G1 (middle) | S0,S1,S2 | Current density versus interdiffusion diffusion length for LO-phonon, BTC and Hybrid QCL design respectively |
| G2 (bottom) | S0,S1,S2 | Emission frequency versus interdiffusion diffusion length for LO-phonon, BTC and Hybrid QCL design respectively |
| Fig3\_Layer\_thickness\_fluctuations.agr | G0 (top) | S0 | Material gain and for the first 100 random layer thickness fluctuations for LO-phonon QCLdesign |
| G1 (middle) | S0 | Material gain and for the first 100 random layer thickness fluctuations for BTC QCLdesign |
| G2 (bottom) | S0 | Material gain and for the first 100 random layer thickness fluctuations for Hybrid QCLdesign |
| G3 (inset top) | S0 | Current density for the first 100 random layer thickness fluctuations for LO-phonon QCLdesign |
| G4 (inset middle) | S0 | Current density for the first 100 random layer thickness fluctuations for BTC QCLdesign |
| G5 (inset bottom) | S0 | Current density for the first 100 random layer thickness fluctuations for Hybrid QCLdesign |
| Fig4a\_Cond\_band\_diffusion\_261K\_LO\_record.agr | G0 | S0, S6, S7 | Bottom of the conduction band potential of the 261 K LO-phonon THz QCL for interdiffusion diffusion lengths $L\_{D}=0, 1.5A, and 3A$  |
| S1-S5 | Wavefunctions squared, 5 states, plotted in light blue |
| Fig4b\_Compositional\_diffusion\_261K\_LO\_record.agr | G0 (top) | S0 | Material gain versus interdiffusion diffusion length for 261 K LO-phonon QCL design  |
| G1 (middle) | S0 | Current density versus interdiffusion diffusion length for 261K LO-phonon QCL design |
| G2 (bottom) | S0 | Emission frequency versus interdiffusion diffusion length for 261 K LO-phonon QCL design |
| Fig4c\_Layer\_variation\_Gain\_Current\_261K\_LO\_record.agr | G0 (top) | S0 | Material gain for all ofthe 81 possible thickness variations for the 261 K record high temperature LO-phonon THz QCL |
| G1 (bottom) | S0 | Current density for all ofthe 81 possible thickness variations for the 261 K record high temperature LO-phonon THz QCL |
| Fig4d\_Single\_layer\_effect\_Gain\_Current\_261K\_LO\_record.agr | G0 (top) | S0-S3 | Material gain forlayer variations of only a single layer for first, second, third and fourth layer respectively in the 261 K record high temperature LO-phonon THz QCL16 |
| G1 (bottom) | S0-S3 | Current density forlayer variations of only a single layer for first, second, third and fourth layer respectively in the 261 K record high temperature LO-phonon THz QCL16 |
| Fig5a\_Cond\_band\_200K\_LO\_phonon.agr | G0 | S0 | Bottom of the conduction band potential of the 200 K LO-phonon THz QCL |
| S1-S6 | Wavefunctions squared, 6 states (left period) |
| S7-S12 | Wavefunctions squared, 6 states (right period) |
| Fig5b\_Cond\_band\_BTC.agr | G0 | S0 | Bottom of the conduction band potential of the BTC THz QCL  |
| S1-S10 | Wavefunctions squared, 10 states (left period) |
| S11-S20 | Wavefunctions squared, 10 states (right period) |
| Fig5c\_Cond\_band\_Hybrid.agr | G0 | S0 | Bottom of the conduction band potential of the Hybrid THz QCL |
| S1-S10 | Wavefunctions squared, 10 states (left period) |
| S11-S20 | Wavefunctions squared, 10 states (right period) |
| Fig5d\_Cond\_band\_261K\_LO\_record.agr | G0 | S0 | Bottom of the conduction band potential potential of the 261 K LO-phonon THz QCL |
| S1-S5 | Wavefunctions squared, 10 states (left period) |
| S6-S10 | Wavefunctions squared, 10 states (right period) |
| Fig6a\_BTC\_Gain\_frequency.agr | G0  | S0-S6 | Material gain $g$ dependence on emission frequency$f$ for electric bias $K=1.7 {kV}/{cm}$, $1.8 {kV}/{cm}, 1.9 {kV}/{cm}, 2.0 {kV}/{cm},$ $2.1 {kV}/{cm}, 2.2 {kV}/{cm}$ and $2.3 {kV}/{cm}$ |
| G1 (inset) | S0 | Emission frequency $f$ of the peaks of material gain $g$ versus the electric bias$K$ for BTC THz QCL |
| Fig6b\_BTC\_transport.agr | G0 | S0 | Material gain $g$ dependence onelectric bias $K$ for BTC THz QCL |
| S1 | Current density $J$ dependence onelectric bias $K$ for BTC THz QCL |

We apologize to the interested reader for the unorthodox storage of the data, but keep in mind that if we provided every individual x-y trace in a separate file, the repository would consist of very large number of files that would be hard to process. In this way, readers can reproduce figures with ease, and get the corresponding figure data by accessing .agr files in text editor.

Kind regards,

The authors