Data information

This repository contains all data that corresponds to figures associated with our publication *“Prospects of temperature performance enhancement through higher resonant phonon transition designs in GaAs-based terahertz quantum-cascade lasers”* and the corresponding Supplementary document (copy is also provided in the repository).

We have used two tools for generating figures in this work: MATLAB and Grace.

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 within .fig (MATLAB) and .agr files. Data extraction from MATLAB figures is straightforward and in many cases we also provided corresponding code that created the figures in the paper and the supplementary document. However, most of our figures are .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-200K.agr | G0 | S0 | $g(T)$ dependance |
| G1 (inset) | S0 | Band structure potential (black) |
| S1 | Ground state wavefunction (green)  |
| S2 | The second state wavefunction (magenta) |
| S3 | The third state wavefunction (red) |
| S4 | The fourth state wavefunction (blue) |
| S5 | The fifth state wavefunction (cyan) |
| S6 | The sixth state wavefunction (cyan) |
| S7 | The seventh state wavefunction (cyan) |
| S8 | The eight state wavefunction (cyan) |
| S9 | Ground state wavefunction in the second period (green) |
| S10 | The second state wavefunction in the second period (magenta) |
| S11 | The third state wavefunction in the second period (red) |
| S12 | The fourth state wavefunction in the second period (blue) |
| S13 | The fifth state wavefunction in the second period (cyan) |
| S14 | The sixth state wavefunction in the second period (cyan) |
| S15 | The seventh state wavefunction in the second period (cyan) |
| S16 | The eight state wavefunction in the second period (cyan) |
| S17-S24 | States 1-8 in the third period (not shown on the graph) |
| fig1b-250K.agr | G0 | S0 | Same as for fig1a-200K.agr |
| G1 (inset) | S0-S24 | Same as for fig1a-200K.agr |
| fig1c-Hybrid.agr | G0 | S0 | Same as for fig1a-200K.agr |
| G1 (inset) | S0-S39 | Similar to fig1a-200K.agr, difference is that S1-S13 correspond to 13 state in one QCL period, S14-S26 to states in the second period, and third period state S27-S39 are not presented in the graph (but data I available in this file). |
| fig1c-Hybrid.agr | G0 | S0 | Same as for fig1a-200K.agr |
| G1 (inset) | S0-S18 | Similar to fig1a-200K.agr, difference is that S1-S6 correspond to 6 states in one QCL period, and other traces correspond to states in adjacent periods. |
| fig1d-Walther.agr | G0 | S0 | Same as for fig1a-200K.agr |
| G1 | S0-S36 | Similar to fig1a-200K.agr, difference is that S1-S12 correspond to 12 states in one QCL period, and other traces correspond to states in adjacent periods. |
| fig1e-Kumar.agr | G0 | S0 | Same as for fig1a-200K.agr |
| G1 (inset) | S0-S21 | Similar to fig1a-200K.agr, difference is that S1-S7 correspond to 7 states in one QCL period, and other traces correspond to adjacent periods. |
| fig1f-Williams.agr | G0 | S0 | Same as for fig1a-200K.agr |
|  | G1 (inset) | S0-S33 | Similar to fig1a-200K.agr, difference is that S1-S11 correspond to 11 states in one QCL period, and other traces correspond to states in adjacent periods. |
| fig2b-LO-phonon.agr | G0 | S0 | $W\_{21}(ΔE\_{21})$ at 10 K (black) |
| S1 | $W\_{21}(ΔE\_{21})$ at 50 K (red) |
| S2 | $W\_{21}(ΔE\_{21})$ at 100 K (blue) |
| S3 | $W\_{21}(ΔE\_{21})$ at 150 K (green) |
| S4 | $W\_{21}(ΔE\_{21})$ at 200 K (magenta) |
| S5 | $W\_{21}(ΔE\_{21})$ at 250 K (maroon) |
| S6 | $W\_{21}(ΔE\_{21})$ at 300 K (dark green) |
| S7 | $W\_{21}(ΔE\_{21})$ at 400 K (purple) |
| G1 (inset) | S0 | $W\_{21}(T)$ for $ΔE\_{21}=14.4 $meV (dotted dark green line) |
| S1 | $W\_{21}(T)$ for $ΔE\_{21}=36$ meV (dotted dark blue line) |
| S2 | $W\_{21}(T)$ for $ΔE\_{21}=50.6 $meV (dotted red line) |
| fig3-W200.agr | G0 | S0 | $W\_{21}(T)$ (dark green) |
| S1 | $W\_{31}(T)$ (blue) |
| S2 | $W\_{41}(T)$ (orange) |
| S3 | $W\_{42}(T)$ (purple) |
| S4 | $W\_{43}(T)$ (red) |
| fig5-newdesigns.agr | G0 | S0 | $g(T)$ for two well design |
| S1 | $g(T)$ for three well design |
| S2 | $g(T)$ for four well design |
| G1 (left inset) | S0-S21 | Similar to fig1a-200K.agr, difference is that S1-S7 correspond to 7 states in one QCL period, and other traces correspond to states in adjacent periods. |
| G2 (right inset) | S0-S24 | Similar to fig1a-200K.agr, difference is that S1-S8 correspond to 8 states in one QCL period, and other traces correspond to states in adjacent periods. |
| supp\_fig\_1b\_gain\_v\_f\_5K | G0 | S0 | $g(f)$ at 18 kV/cm (black) |
| S1 | $g(f)$ at 19 kV/cm (red) |
| S2 | $g(f)$ at 20 kV/cm (blue) |
| S3 | $g(f)$ at 21 kV/cm (purple) |
| S4 | $g(f)$ at 22 kV/cm (dark green) |
| S5 | $g(f)$ at 23 kV/cm (brown) |
| G1 (inset) | S0 | $f\left(K\right)$ (magenta) |
| supp\_fig\_3\_g\_v\_K\_multi\_T.agr | G0 (left y axis) | S0 | $g(K)$ at 5K (black) |
| S1 | $g(K)$ at 55K (red) |
| S2 | $g(K)$ at 115K (blue) |
| S3 | $g(K)$ at 165K (purple) |
| S4 | $g(K)$ at 225K (dark green) |
| G1 (right y axis) | S0 | $J(K)$ at 5K (black) |
| S1 | $J(K)$ at 55K (red) |
| S2 | $J(K)$ at 115K (blue) |
| S3 | $J(K)$ at 165K (purple) |
| S4 | $J(K)$ at 2255K (dark green) |
| AppFig1a-200K\_comp.agr | G0 (left y axis) | S0 | $J(K)$ at 20K (blue) of structure in ref [46] |
| S1 | $J(K)$ at 20K (blue) of improved structure based on structure in ref [46] |
| G1 (right y axis) | S0 | $L(K)$ at 20K (dashed red) of structure in ref [46] |
| S1 | $L(K)$ at 20K (dashed blue) of improved structure based on structure in ref [46] |
| AppFig1b-Hybrid.agr | G0 (left y axis) | S0 | $J(K)$ at 20K (blue) of structure in ref [15] |
| S1 | $J(K)$ at 20K (blue) of improved structure based on structure in ref [15] |
| G1 (right y axis) | S0 | $L(K)$ at 20K (dashed red) of structure in ref [15] |
| S1 | $L(K)$ at 20K (dashed blue) of improved structure based on structure in ref [15] |
| AppFig1c-Assisted.agr | G0 (left y axis) | S0 | $J(K)$ at 20K (blue) of structure in ref [47] |
| S1 | $J(K)$ at 20K (blue) of improved structure based on structure in ref [47] |
| G1 (right y axis) | S0 | $L(K)$ at 20K (dashed red) of structure in ref [47] |
| S1 | $L(K)$ at 20K (dashed blue) of improved structure based on structure in ref [47] |
| AppFig1d-Double.agr | G0 (left y axis) | S0 | $J(K)$ at 20K (blue) of structure in ref [48] |
| S1 | $J(K)$ at 20K (blue) of improved structure based on structure in ref [48] |
| G1 (right y axis) | S0 | $L(K)$ at 20K (dashed red) of structure in ref [48] |
| S1 | $L(K)$ at 20K (dashed blue) of improved structure based on structure in ref [48] |

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, especially for wavefunction insets in Figure 1 and Figure 5.

 In this way, readers can reproduce figures with ease, and get the corresponding figure data by accessing .agr files in text editor.

The list of MATLAB figures and files is:

|  |  |
| --- | --- |
| Filename | Description |
| fig2a-W21\_3D.fig | Three-dimensional representation of scattering rate dependence on state separation. Data can be exported in MATLAB when opening the figure.  |
| fig4-improve.figfig4-improve.m | MATLAB figure and the corresponding code used for its creation for figure 4 in the paper. |
| supp\_fig\_1a\_gain\_v\_f\_K\_5K.fig | Three dimensional representation of material gain dependence on frequency and electrical bias when lattice temperature is fixed at 5 K, that corresponds to fig1a in supplementary file. The data can be extracted from the figure in MATLAB, however we also provide data file and the corresponding code for its creation (see below). |
| supp\_fig\_2a\_gain\_v\_T\_K.fig | Three dimensional representation of material gain dependence on temperature and electrical, that corresponds to fig2a in supplementary file. The data can be extracted from the figure in MATLAB, however we also provide data file and the corresponding code for its creation (see below). |
| supp\_fig\_2b\_current\_v\_T\_K.fig | Three dimensional representation of current density dependence on temperature and electrical, that corresponds to fig2a in supplementary file. The data can be extracted from the figure in MATLAB, however we also provide data file and the corresponding code for its creation (see below). |
| Gvf.datGrvf\_pol\_3D.datJrvf\_3D.datplot3D.m | These files correspond to data used to generate supp\_fig1 and supp\_fig2 in the supplementary data. Code that reads .dat files and generates the figures is plot3D.m, Gvf.dat corresponds to supp\_fig1a, Grvf\_pol\_3D.dat to supp\_fig2a and Jrvf\_3D.dat to supp\_fig2b. |

Kind regards,

The authors