Data information

This repository contains all data that corresponds to figures associated with our publication *“Resonant tunnelling and intersubband optical properties of ZnO/ZnMgO semiconductor heterostructures: impact of doping and layer structure variation”*.

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 |
| Fig1\_potential.agr | G0 | S0-S5 | Wavefunctions, 6 states, plotted in red |
| S6 | Bandstructure potential (full black line) when Hartee and exchange correlation is taken into account |
| S7 | Bandstructure potential (dashed black line) when Hartee and exchange correlation is not taken into account |
| Fig2\_alpha.agr | G0 (top) | S0, S1, S2 | Absorption coefficient with depolarization effect for $N\_{D}=3⋅10^{18}, 3⋅10^{19}$ and $5⋅10^{19} cm^{-3}$, respectively |
| G1 (bottom) | S0, S1, S2 | Absorption coefficient without depolarization effect for $N\_{D}=3⋅10^{18}, 3⋅10^{19}$ and $5⋅10^{19} cm^{-3}$, respectively |
| Fig3\_Emax\_Nd\_loglog.agr | G0 (main) | S0 | Peak energy without depolarization effect (blue) |
| S1 | Peak energy with depolarization effect (red) |
| G1 (inset) | S0 | Absorption coefficient without depolarization effect (blue) |
| S1 | Absorption coefficient with depolarization effect (red) |
| Fig4\_x.agr | G0 (main) | S0-S5 | Absorption coefficient vs E for x=10,11,12,13,14,15 %, respectively  |
| G1 (inset) | S0 | Emax vs x (purple). |
| Fig5\_dW.agr | G0 | S0-S8 | Absorption vs E as well width is varied from -10 A to 10 A with step of 2.5 A (9 traces in total). |
| G1 (inset) | S0 | Emax vs well width (purple) |
| Fig6\_Potential\_concentration\_Wb=18\_n=3e18.agr | G0 (top) | S0,S1,S2 | Bandstructure potential profile for $V\_{R}$=0, 0.08 and 0.15 V, respectively |
| G1 (bottom) | S0,S1,S2 | Concentration profile for Vr=0, 0.08 and 0.15 V, respectively |
| Fig7\_varying\_n\_Wb=18.agr | G0 (main graph) | S0,S1,S2 | $J(V\_{R})$ dependence for $N\_{D}=5⋅10^{17}, 1⋅10^{18}$ and $5⋅10^{18} cm^{-3}$ , respectively |
| G1 (top inset left y axis) | S0 | PVR vs $N\_{D}$ profile |
| G2 (top inset right y axis) | S0 | $ΔJ$ vs $N\_{D}$ profile |
| G3 (bottom inset) | S0 | $U\_{NDR}$ vs $N\_{D}$ profile |
| Fig8\_varying\_Wb\_n=3e18.agr | G0 (main graph) | S0,S1,S2 | $J(V\_{R})$ dependence for $W\_{B}=1.3, 1.8$ and $2.3 nm$ , respectively |
| G1 (inset left y axis | S0 | PVR vs $W\_{B}$ profile |
| G2 (inset right y axis) | S0 | $ΔJ$ vs $W\_{B}$ profile |
| Fig9\_varying\_x\_Wb=1.3\_n=1e18.agr | G0 (main graph) | S0,S1,S2 | $J(V\_{R})$ dependence for $x=8, 12$ and $14 \%$ , respectively |
| G1 (inset left y axis | S0 | PVR vs $x$ profile |
| G2 (inset right y axis) | S0 | $ΔJ$ vs $x$ profile |

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