



HIERN 48 wellplate spectral fitting program manual

Version 1.0.0

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1 Introduction

The "**HIERN 48 wellplate spectral fitting program**" was designed to facilitate the evaluation of measurement data obtained from a 48 sample wellplate as used with Tecan. Typically the file types are supported in the original format as given by the instruments present at HIERN. The program is capable of evaluating five different types of measurements:

1. **Photoluminescence spectra** either from StellarNet or Tecan spectrometer
2. **Photoluminescence excitation spectra** from Tecan spectrometer
3. **reflectance spectra** from StellarNet spectrometer
4. **Raman spectra**
5. **time-resolved photoluminescence spectra**

For each of these methods a correction depending on a reference and the type of measurement is performed. Afterwards the corresponding fits are performed and the fit parameters exported to output files in the previously chosen folder. Those files are named automatically and will be overwritten if the program is used in the same folder again. By plotting the results the plot is generated and simultaneously saved into the same folder as the fit results. All results are saved as .csv, .txt, .png or respectively .mp4 files and named automatically.

2 Main User Interface

After opening the Program the User Interface looks as shown in fig. 1. It offers five different measurement methods. Some of those methods feature more than one fitting program (PL and trPL).

In fig. 1 the different methods are marked as red boxes. In general a fitting method consists of:

1. **start button** for data import (green)
2. at least one **2D plot button** (turquoise)
3. and **3D plot buttons** (lime)

By clicking the start button any previous calculations, plots and settings (e.g. well selection) are deleted if not saved as output files.

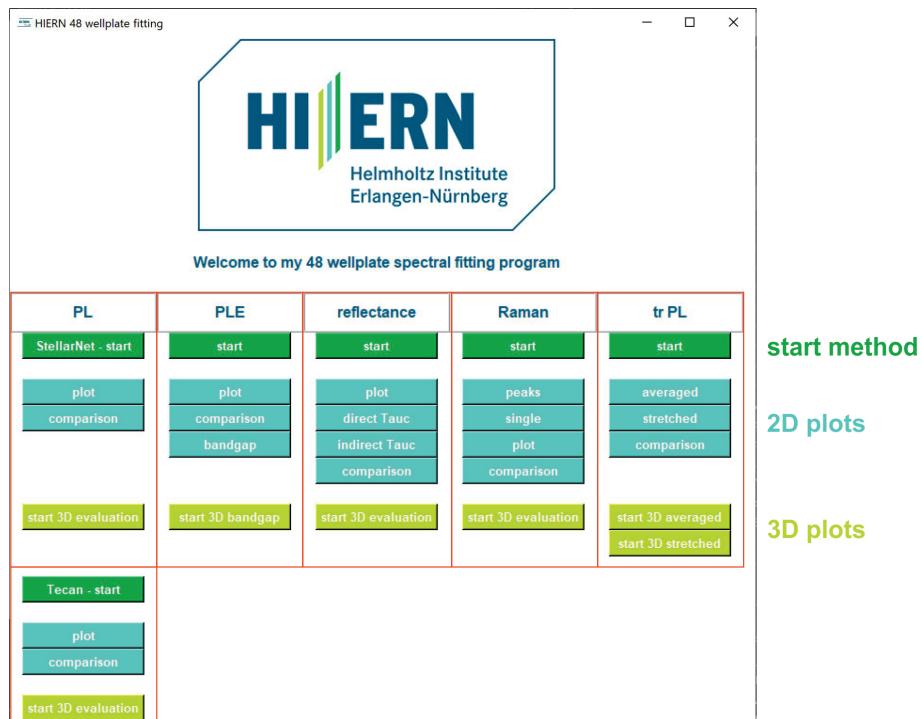


Figure 1: Main User Interface with red boxes indicating methods

3 Methods

3.1 Photoluminescence spectra

StellarNet PL The StellarNet PL User Interface consists of two steps:

1. **well selection:** allows the user to choose for which positions of a standard 48 wellplate measurement data should be evaluated. The buttons turn lime when chosen and grey when unchosen again.
2. **file dialog:** allows the user specifically for each method to choose the corresponding reference file, measurement data files and the result folder. After selecting the correct number of files, the buttons turn grey. More specific for each method as the user is choosing the reference file, the measurement data files and the results folder. After clicking and choosing the right number of files the buttons turn grey. The number of chosen wells is also displayed in this dialog.

(a) well selection

(b) file dialog

Figure 2: StellarNet PL two step User Interface

For the StellarNet PL fitting method the files should match the standards as provided by the StellarNet setup:

1. A single file for every measurement with two columns for the x- and y-data separated by spaces.
2. The x-axis should be in units of wavelength and will be converted to eV.

The measurement files should be ordered according to the order of the wellplate (A1, ..., A8, B1, ..., C1, ..., D1, ..., E1, ..., F1, ..., F8) as they are read in according to this order (fig. 3).

Name	Änderungsdatum	Typ	Größe
results	08.04.2022 15:39	Dateiordner	
A1.SSM	08.04.2022 14:16	SSM-Datei	39 KB
A2.SSM	08.04.2022 14:16	SSM-Datei	39 KB
A3.SSM	08.04.2022 14:16	SSM-Datei	39 KB
A4.SSM	08.04.2022 14:17	SSM-Datei	39 KB
A5.SSM	08.04.2022 14:17	SSM-Datei	39 KB
A6.SSM	08.04.2022 14:17	SSM-Datei	39 KB
A7.SSM	08.04.2022 14:18	SSM-Datei	39 KB
A8.SSM	08.04.2022 14:18	SSM-Datei	39 KB
B1.SSM	08.04.2022 14:20	SSM-Datei	39 KB
B2.SSM	08.04.2022 14:19	SSM-Datei	39 KB
B3.SSM	08.04.2022 14:19	SSM-Datei	39 KB
B4.SSM	08.04.2022 14:19	SSM-Datei	39 KB
B5.SSM	08.04.2022 14:19	SSM-Datei	39 KB
B6.SSM	08.04.2022 14:19	SSM-Datei	39 KB
B7.SSM	08.04.2022 14:18	SSM-Datei	39 KB
B8.SSM	08.04.2022 14:18	SSM-Datei	39 KB
C1.SSM	08.04.2022 14:20	SSM-Datei	39 KB
c2.SSM	08.04.2022 14:20	SSM-Datei	39 KB
C3.SSM	08.04.2022 14:20	SSM-Datei	39 KB
C4.SSM	08.04.2022 14:20	SSM-Datei	39 KB
C5.SSM	08.04.2022 14:21	SSM-Datei	39 KB
C6.SSM	08.04.2022 14:21	SSM-Datei	39 KB
C7.SSM	08.04.2022 14:21	SSM-Datei	39 KB
C8.SSM	08.04.2022 14:21	SSM-Datei	39 KB
D1.SSM	08.04.2022 14:23	SSM-Datei	39 KB
D2.SSM	08.04.2022 14:22	SSM-Datei	39 KB

Figure 3: Example of sorted and ideally named files and result folder

The read in data are corrected according to the given reference file (eq. (1)).

$$PL_{\text{corrected}} = PL_{\text{data}} - \frac{\text{reference}_{\text{data}}}{(\text{reference}_{\text{data}_{\text{peak}}} \cdot PL_{\text{data}_{\text{peak}}})} \quad (1)$$

After all corrections the curves are each fitted with a single Gaussian function (eq. (2)) and also all curves and fits are normalized.

$$f(x; A, \mu, \sigma) = \frac{A}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad (2)$$

$$fwhm = 2\sigma\sqrt{2\ln 2} \quad (3)$$

You can click the "plot" button to display the corresponding plots (fig. 4).

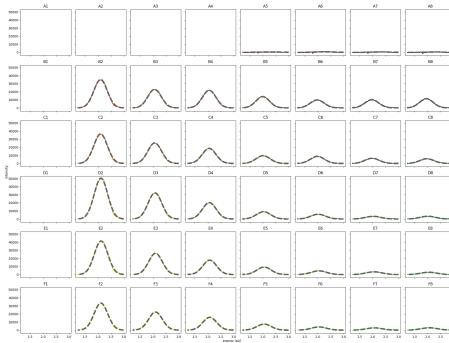


Figure 4: plot button result

Additionally you can click the "comparison" button to open a pop-up window (fig. 5a) asking for a row and column of your 48 wellplate. The graphs and fits of this row and column are stacked in two plots (fig. 5b) and saved under the corresponding name e.g. "row_E_column_2.png".

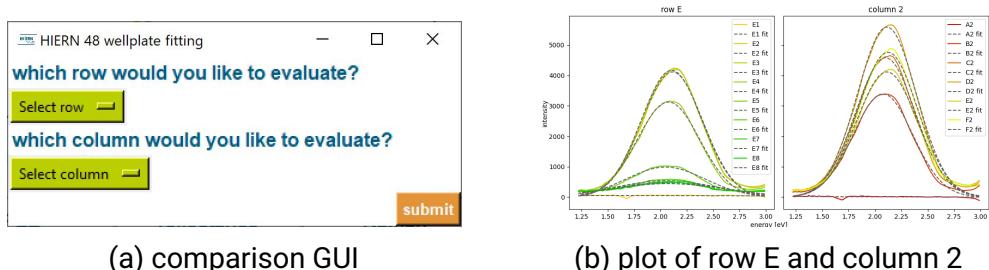


Figure 5: comparison button

By clicking the "start 3D evaluation" button you open another pop-up window (fig. 6a) which asks for the desired front position (fig. 6b) of the 3D plot image and also for the alignment of the 3D plots (horizontal or vertical). The alignment can be switched by clicking on the "horizontal" (or respectively "vertical") button. After clicking submit an animated 3D plot of the fitting parameters (fwhm (eq. (3)), amplitude, height and center) is generated.

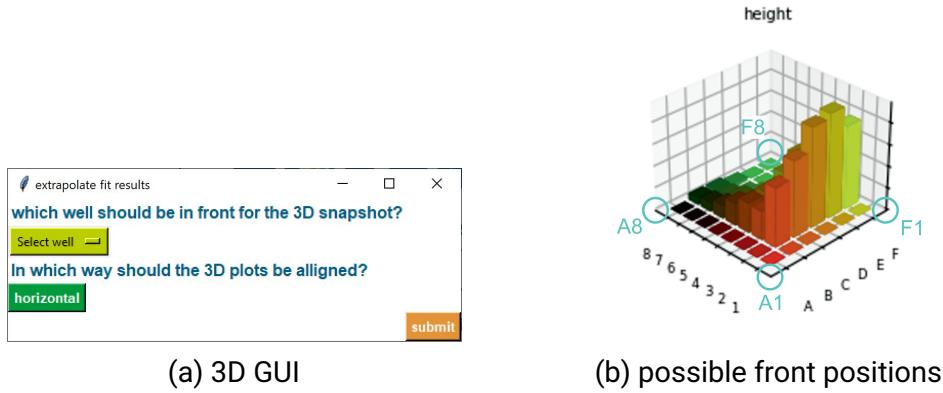


Figure 6: 3D plot options

A snapshot of this video is also saved as an image (fig. 7). All plots are simultaneously saved as images or .mp4 videos but can also be zoomed in and saved again from the pop-up window.

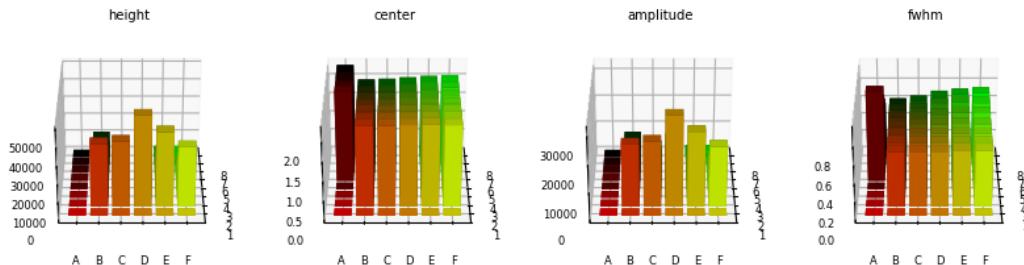


Figure 7: 3D PL plot

For the 3D plots the underlying data tables are also saved as .csv files both individually for each parameter (center, amplitude, height, fwhm) and once as a summary (e.g. table 1).

<i>fwhm</i>	1	2	3	4	5	6	7	8
A	2.73	0.17	0.25	2.88	0.15	0.43	0.15	2.37
B	3.24	0.63	0.64	0.63	0.62	0.63	0.63	0.63
C	1.46	0.62	0.63	0.62	0.62	0.64	0.63	0.65
D	0.47	0.62	0.62	0.62	0.63	0.63	0.63	0.63
E	0.54	0.62	0.62	0.62	0.62	0.63	0.63	0.63
F	0.59	0.62	0.62	0.62	0.62	0.63	0.63	0.63

Table 1: Autogenerated table from .csv file.

Tecan PL

The program for the Photoluminescence spectra obtained from the Tecan spectrometer is working quite similar to the one for StellarNet PL measurements.

The user interface consists of the two steps **well selection** and the **file dialog** requires just one data file (.txt) and the result folder. This file should contain the x-data (e.g. header: Wavel.) in the first column and one more tabulator separated data column for each measured sample (e.g. header: A1, ...) in the right order. The x-data should be in units of wavelength and will be converted to energy units (eV) accompanied by an Jacobian correction (eq. (4)).

$$PL_{corrected}(E) = PL_{corrected}(\lambda) \frac{d\lambda}{dE} \quad (4)$$

3.2 Photoluminescence Excitation spectra

The PLE program also consists of a similar two step user interface as the Tecan PL program. You choose the wells of the 48 plate and afterwards provide one measurement data file (.txt) and a result folder. The measurement data file should have the following structure: first column x-data in units of wavelength (e.g. header: Wavel.) , one additional tabulator separated column for each selected well (e.g. header: A1, ...) in the right order. Afterwards the data are corrected with the Jacobian correction (eq. (4)) as for the PL spectra. The fitting is performed using the same Gaussian function (eq. (2)) as for PL. Those plots can be displayed by the plot button. The comparison button offers the same features as for the PL methode (fig. 5).

Click the turquoise "bandgap" button to get the linear fits for the bandgap extrapolation displayed. For this fit the low-energy site of the Gaussian curve is fitted according to eq. (5) and the bandgap extrapolated as the x-axis intercept (eq. (6)) of this plot.

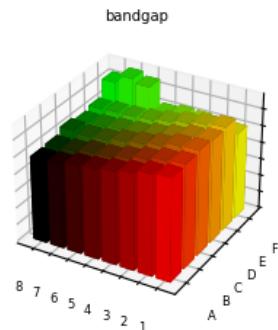
$$y = mx + t \quad (5)$$

$$x_0 = -\frac{t}{m} \quad (6)$$

Use the button "start 3D evaluation" to show the fit parameters from the Gaussian fit as a 3D plot and the button "start 3D bandgap" to show an animated 3D plot of the calculated bandgaps (fig. 8 which is also saved as a snapshot).



(a) bandgap button result



(b) start 3D bandgap button result

Figure 8: PLE bandgap plots

3.3 Reflectance spectra

The reflectance program features a two step user interface: well selection and file dialog. A reference file, a measurement file for every position and a result folder must be provided. All files must contain two columns with the x-data in the first and y-data in the second separated by spaces. There has to be one file for each chosen well. The spectra are calculated according to eq. (7) and the wavelength x-axis is changed to an energy x-axis.

$$\text{reflectance}_{\text{corrected}} = \frac{\text{reference}_{\text{data}}}{\text{reflectance}_{\text{data}}} \quad (7)$$

The plot button displays the calculated spectra and saves the plot in the previously chosen folder. With the comparison button the plots can be stacked as for PL and PLE spectra but no fit is added in these images.

Additionally the bandgaps both for a direct and an indirect semiconductor are estimated according to the Tauc plot (eq. (10)) using the Kubelka-Munk function (eq. (8) and eq. (9)):

$$R = \frac{R_{\text{sample}}}{R_{\text{reference}}} \cdot \frac{1}{100} \quad (8)$$

$$F(R) = \frac{K}{S} = \frac{(1 - R)^2}{2R} \quad (9)$$

$$(F(R)h\nu)^{\frac{1}{\gamma}} = B(h\nu - E_g) \quad (10)$$

with $\gamma = 0.5$ for direct and $\gamma = 2$ for indirect semiconductors.

The curves are than correspondingly fitted with a linear function (eq. (5)) and the x-axis intercept (eq. (6)) is interpreted as an estimate for the bandgap energy.

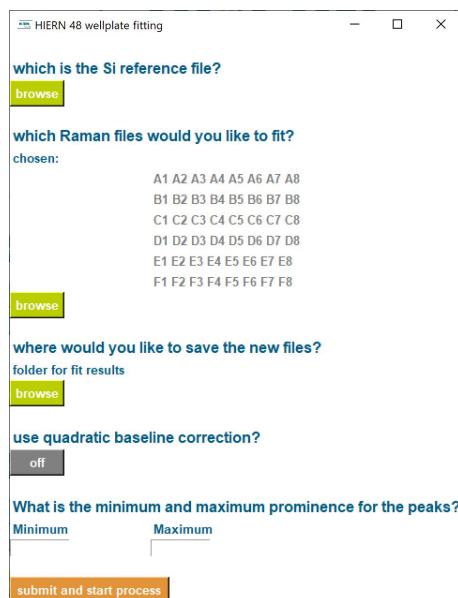
You can display and simultaneously save the corresponding plots with the buttons "Tauc direct" and "Tauc indirect". By clicking the "start 3D evaluation" button two animated 3D plots showing the calculated direct and indirect bandgap values are produced and a .mp4 video and a .png snapshot saved at the same time.

3.4 Raman spectra

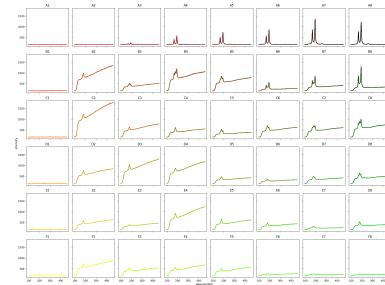
The Raman method features a two step user interface using the well selection and a file dialog. A Silicon Raman measurement has to be chosen as a reference. For each measured sample an individual file has to be provided. Finally a result folder is necessary.

All files have to consist of two columns (one for x- and one for y-data) separated with a tabulator.

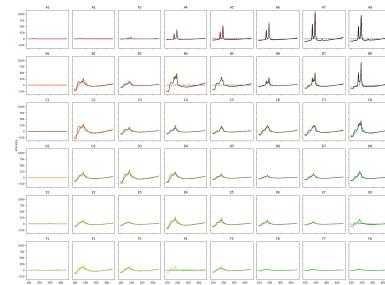
Additionally a quadratic baseline correction can be switched on (fig. 9c) and off (fig. 9b, default: off) and the peak minimum and maximum prominence has to be chosen. The prominence of a peak measures how much a peak stands out from the surrounding baseline of the signal and is defined as the vertical distance between the peak and its lowest contour line. A starting condition could be using 0.3 for the minimum and 90 for the maximum value.



(a) Raman file dialog



(b) without quadratic baseline correction



(c) with quadratic baseline correction

Figure 9: Raman file dialog and baseline effects

From the reference file the single peak is extracted and its deviation from the literature value of 521 cm^{-1} [1] is calculated. This shift is afterwards added to the x-data column of the given Raman measurement files.

All Raman spectra are first scanned for their peaks. Those peak positions can be shown by the "peak" button (result shown in fig. 11a). Afterwards depending on the number of peaks the spectra are fitted by one linear and

various Lorentzian fits (eq. (11)).

$$f(x; A, \mu, \sigma) = \frac{A}{\pi} \left[\frac{\sigma}{(x - \mu)^2 + \sigma^2} \right] \quad (11)$$

Those fits can be viewed for each well individually using the "single" button.

CAUTION: These plots are not saved automatically!

By clicking the "save" button in the corresponding pop-up window (fig. 10a) the plot is saved in the previously chosen folder under the wellname (e.g. "single_fit_of_C3.png"). Here every single Lorentzian is shown explicitly (fig. 10b).

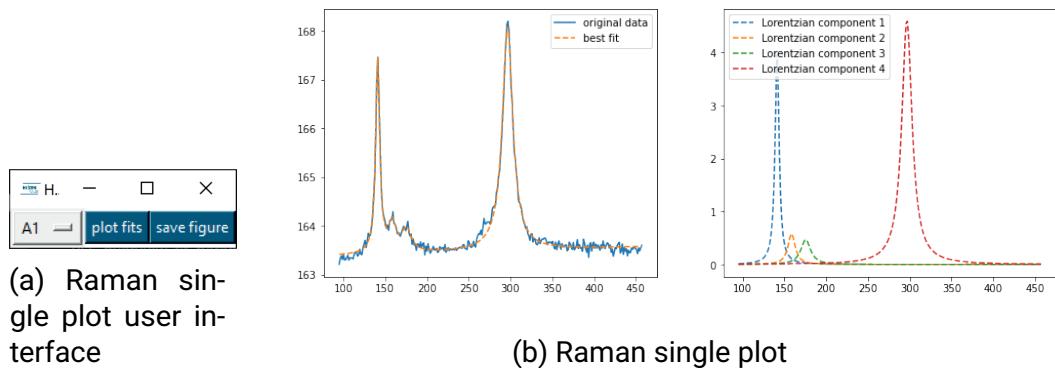


Figure 10: Raman single button results

Alternatively all fits can be plotted at once in the 8x6 order using the "plot" button (fig. 11b). This fit is saved again automatically. For each data set only the summed up fit is displayed. The comparison button also stacks the chosen graphs but again without any fits.

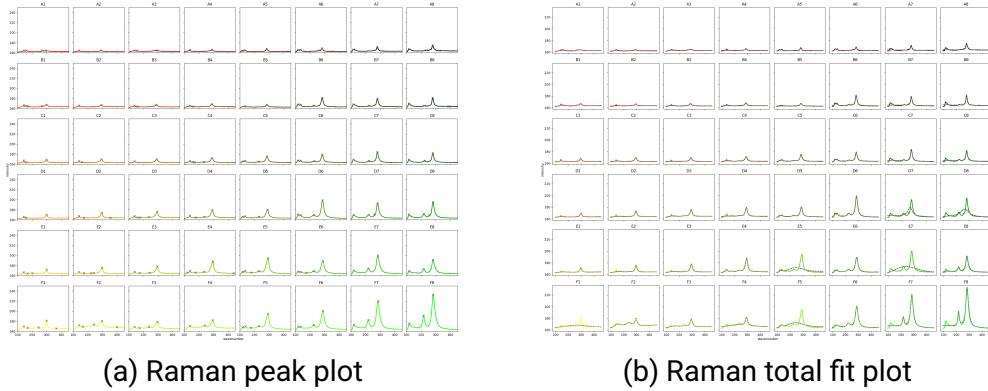


Figure 11: Raman 8x6 plots

By clicking the "3D evaluation" button a new window (fig. 12a) pops up asking for three entries:

- **the start- and endvalue of an interval:** used to evaluate the fit parameters for peaks whose center lies in the interval range in each of the data sets
- **the name:** used for both the titles in the video/image and the file name (fig. 12b, "3D_animation_A1g.png")

CAUTION: The .csv files from the 3D plot are not saved by customized names but by standardized ones so by redoing the plot they are overwritten!

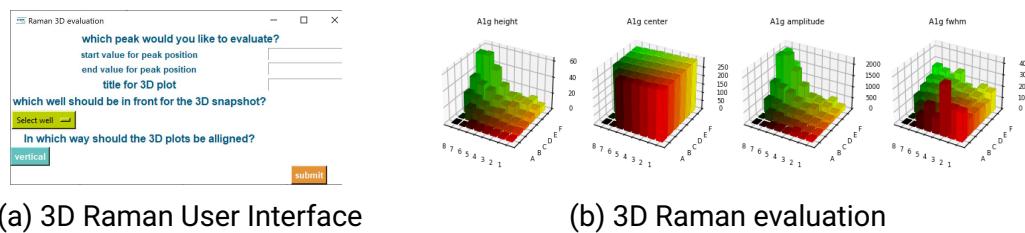


Figure 12: 3D Raman dialog and result

3.5 time-resolved Photoluminescence spectra

The user interface consists of the well selection and the file dialog. You have to choose one file for each measured sample, a result folder and also the fitting method.

For each data file the first 87 rows containing metadata are skipped and then the file should contain two tabulator separated columns with x- and y-data. For time-resolved photoluminescence spectra not only the wells and data have to be selected by the user but also the fitting method. The fit can be either performed using a three exponential function (eq. (12)) and afterwards averaging the lifetime (eq. (13)) or using a stretched exponential function (eq. (14)) which not only gives the lifetime but also a heterogeneity parameter (b).

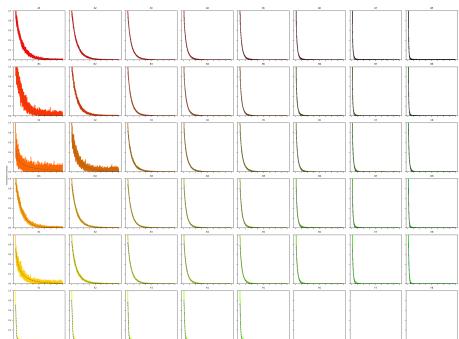
$$f(x; A_1, \tau_1, A_2, \tau_2, A_3, \tau_3) = A_1 e^{-\frac{x}{\tau_1}} + A_2 e^{-\frac{x}{\tau_2}} + A_3 e^{-\frac{x}{\tau_3}} \quad (12)$$

$$t = \frac{\sum A_i \tau_i^2}{\sum A_i \tau_i} \quad (13)$$

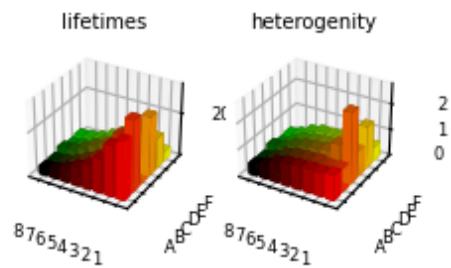
$$f(x; \tau, b) = e^{-(\frac{x}{\tau})^b} \quad (14)$$

For either method the initial data points before the start of the luminescence are cut off and then the curves are normalized.

The plot commands (both 2D and 3D) are separated for the two fit methods. So after choosing the averaged three exponential function for fitting you have to press the corresponding buttons (averaged and start 3D averaged) for the plots and vice versa for the stretched exponential function. An example of those plots is shown in fig. 13. Independently of the chosen fit methods the measurement curves can be shown in a comparison but without a fit curve by using the comparison button.



(a) trPL stretched plot



(b) trPL 3D plot result

Figure 13: trPL plots

References

- [1] Wen-Jen Lee and Yong-Han Chang. "Growth without Postannealing of Monoclinic VO₂ Thin Film by Atomic Layer Deposition Using VCl₄ as Precursor". In: *Coatings* 8 (Nov. 2018), p. 431. DOI: [10.3390/coatings8120431](https://doi.org/10.3390/coatings8120431).