ReadMe GUI_FitSCLC

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Contents

1. Required documents

To run the application, the following documents are needed:

Stand-alone application:

- GUI_FitSCLC.exe
- MatLab runtime (not included here, can be downloaded for free from the MatLab website, it's about 3 GB large but does not require a license).

In MatLab:

- GUI_FitSCLC.fig (figure file containing the GUI)
- GUI_FitSCLC.m (main program handling all actions in the GUI)
- FitSCLCerror.m
- FreeFit.m
- Gill.m
- mu0_T.m
- ODDD.m
- Pasveer.m
- SCLC.m
- SetActive.m.

2. Running the program

The exe-file runs like a normal executable. To run the program in MatLab, all required files should sit in a single directory that is made the active directory of MatLab. Either opening the GUI_FitSCLC.fig file in GUIDE or opening GUI_FitSCLC.m in the editor and pressing the green arrow should get you going. In both cases this GUI will appear (Figure 1):

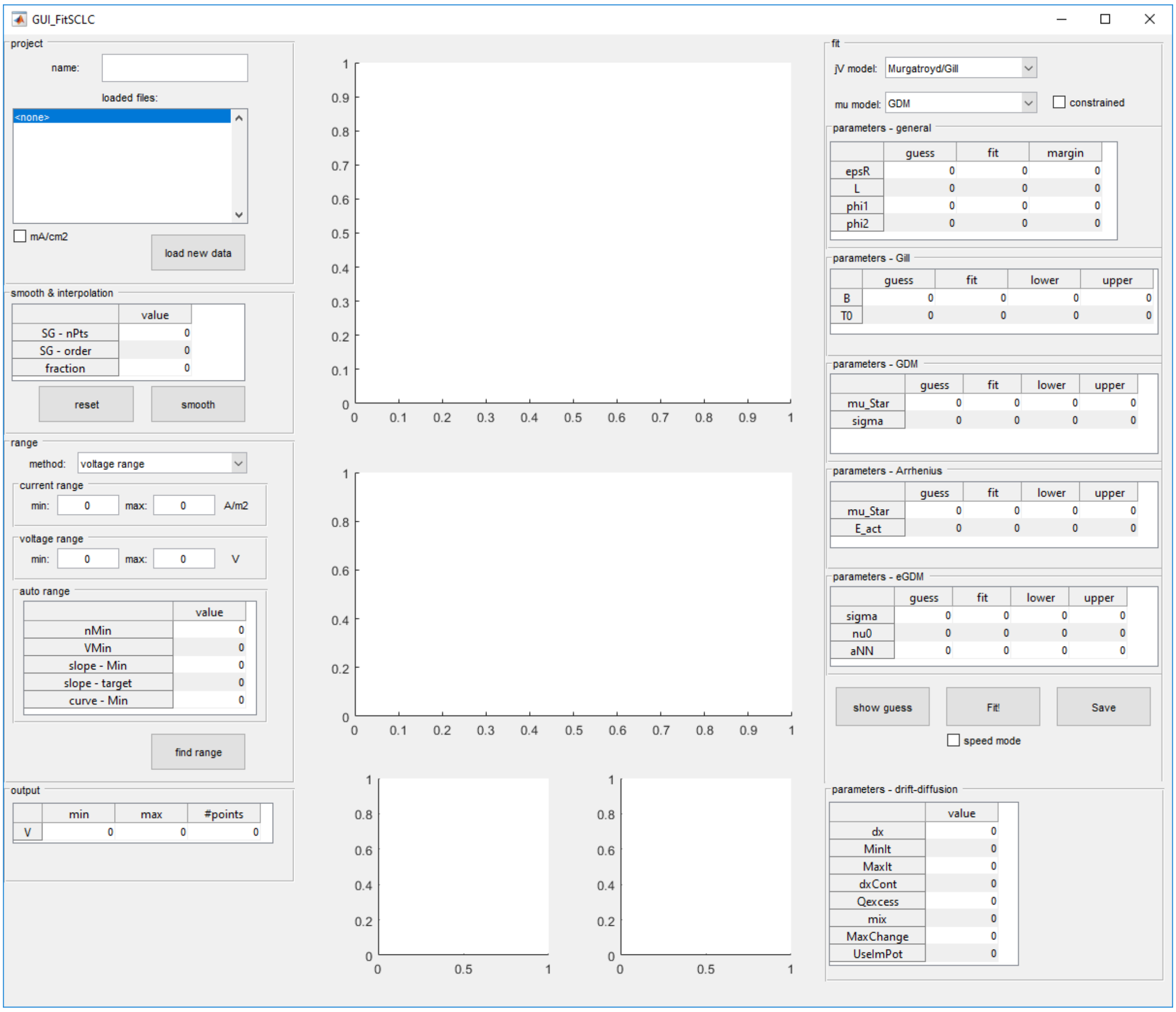


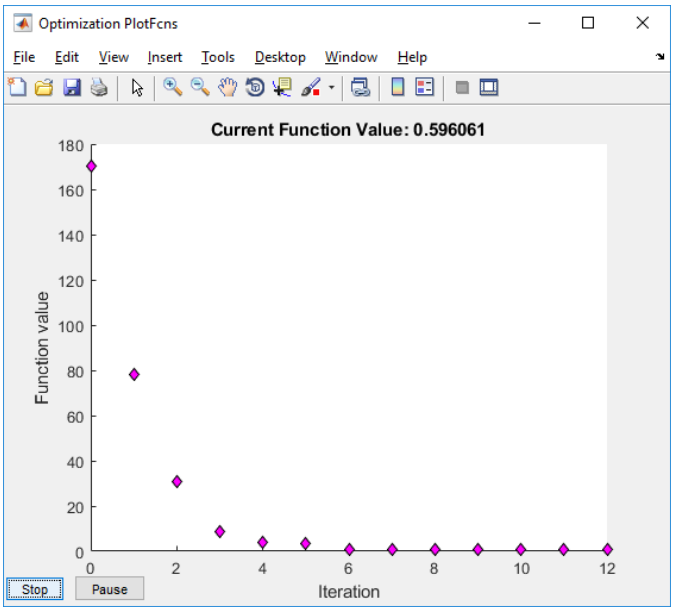
Figure 1. GUI as shown on opening the program

To fit your JV data, you'll have to go through a number of steps that are organized counter-clockwise, starting on the upper left of the GUI:

1. Define a project name. The name will also be used to store all output in the same folder as from where the data are loaded, see also steps 2, 9.
2. Load some data. The program expects a CSV file with V (in Volts) in the first column and J (in A/m^2 or mA/cm^2, use the toggle in the GUI to indicate) in the second. **The filename should end in …xxxK.txt, with xxx three (!) digits defining T in K.**
   The loaded data will be displayed in the upper two graph windows, the upper being the JV curves, whereas the middle panel shows the corresponding power law slope $d(\log(J))/d(\log(V))$.
   IMPORTANT: each JV can contain up to 10 000 data points, but more points lead to slower fitting.
3. Optional: smooth the data. This only affects/helps the auto-range procedure. The results are shown as thin dashed lines.
4. Select the data range to be fitted using one of the methods in the pull-down menu and the corresponding parameters.
5. Set the voltage range for which the fitted JV curves are calculated. When 'speed mode' is used (only active/visible for Drift-Diffusion/eGDM), these are also the points at which trial

JV's are calculated in which case the choice of voltage points has influence on both the speed and the accuracy of the fit (speed mode enables faster fitting at marginally lower accuracy).

6. Select the model to fit the data to from the pull-down menus and set the trial parameters and the allowed range of variation. To help with that, the 'show guess' button plots the JV's corresponding to the chosen guess parameters.
   IMPORTANT: for some parameters that usually take either very small or very large values (B, mu_Star, nu0), the upper and lower limits are to be read as exponents. E.g. -2 and +2 imply the upper and lower limit are 10^{-2} and 10^{2} times the guess value.
   IMPORTANT: to avoid landing in some local minimum, it is a good idea to run the fit several times, each time with different guess parameters.
7. Fit and inspect the result. When pressing fit, a new window will open, showing the progress of the least squares routine. More concretely, the plot will show the least-squares error:



8. At any time, the procedure can be stopped with the 'stop' button and the program will use the best (not converged!) fit till then. Otherwise, another small window will appear when the fitting is complete. The fitted JV's and slopes will be plotted, and the corresponding parameters will be added to the relevant table(s). For the Murgatroyd/Gill fits, also an analysis of the μ_0 and γ vs. T will be made and plotted in the lower two graph windows.
   IMPORTANT: check that the fitted parameter values are not constrained by the upper and lower limits, unless this is desired.
9. Save the data. The program saves the following in the same directory as from which the JV curves come:
   - '[project name] par.txt': text file with guess and fit values of the parameters used in the last saved fit
   - '[project name] mu_gamma.txt': text file with the fitted zero-field, zero-density mobility μ_0 and (when applicable) the field-enhancement factor γ vs. T.
   - '[project name] jV fit.txt': text file with fitted JV curves, first line contains T.
   - '[project name] slope fit.txt': text file with corresponding slope curves, first line contains T.
   - '[project name] all.mat': MatLab file containing 3 structures with experimental data, the used input parameters (from the GUI) and the fitting results.

10. It seems that sometimes the program freaks out. Usually it indicates bad input, but if nothing helps, restarting will.
    The drift-diffusion model is not as stable (and not as fast) as the analytical models, especially when the injection barriers are low and/or when the image potential is activated (UseImPot=1). It might show up as a failure to make progress in the fitting routine or failure to plot (parts of) the JV curves when pressing 'show guess'. To solve the problem, either deactivating the image potential, or (a) reducing the weight factor of old and new solutions in the self-consistent loop ('mix') or (b) reducing the allowed excess charge ('Qexcess' is the maximum ratio of the actual charge in the device and the charge expected on basis of the geometrical capacitance) or (c) changing the mesh size ('dx') might help.

After this procedure the GUI might look something like this (figure 2):

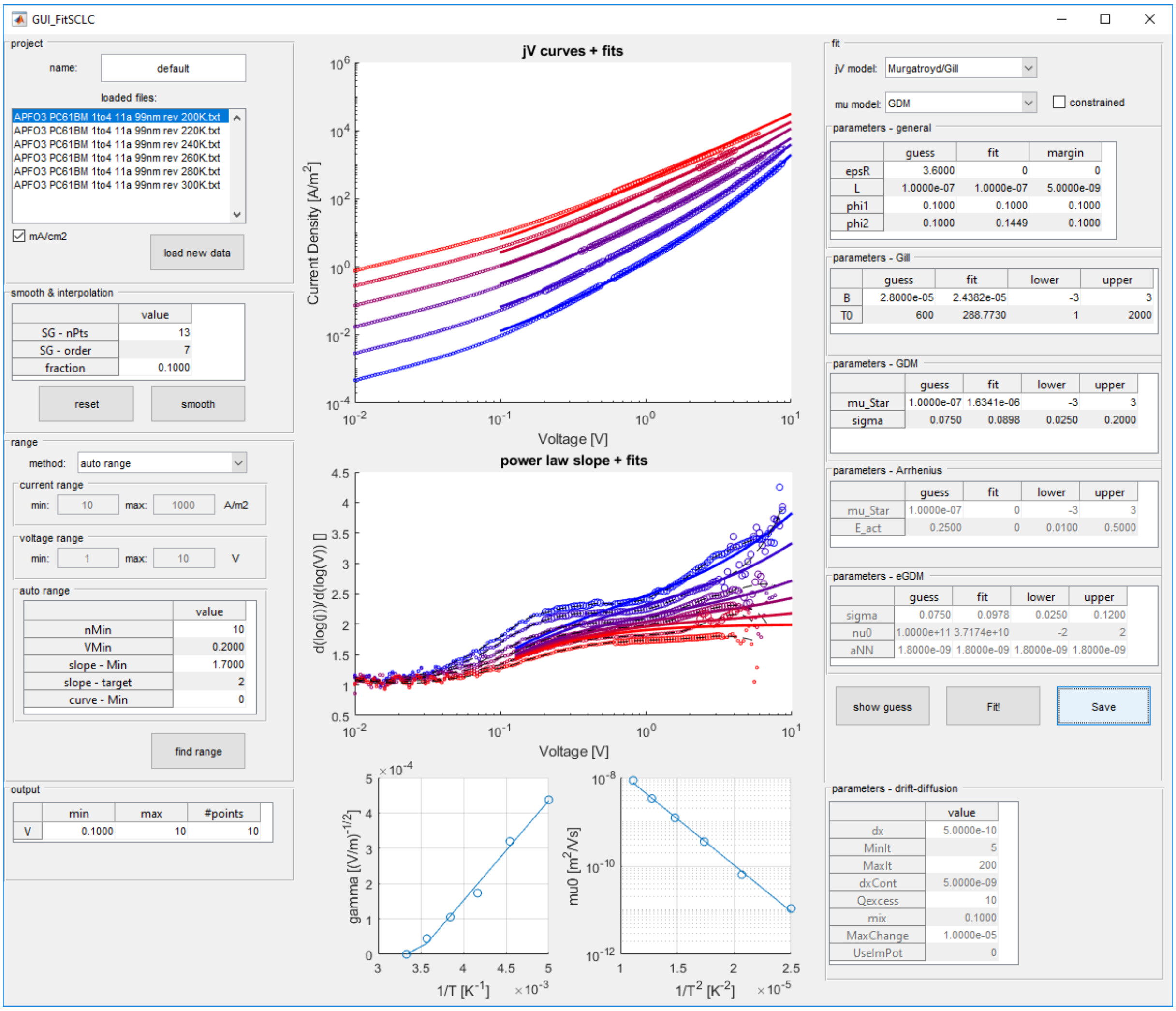


Figure 2. GUI after a completed fitting procedure.

3. Some general remarks

- The program uses SI units throughout the GUI, with energies being measured in eV. Parameter units are not shown for lack of space.
- Hovering the mouse over buttons and input fields will bring up a tooltip.

- The Murgatroyd/Gill model uses a built-in voltage V_{bi}, the drift-diffusion model uses two input barriers (phi1, phi2). To keep the GUI consistent, only φ_1 and φ_2 are shown. They are related to V_{bi} via $V_{bi} = \varphi_1 - \varphi_2$. For the Murgatroyd/Gill model only the difference matters, for drift diffusion the actual values matter!
- To make a new executable in MatLab (requires the compiler 'mcc'), type: "mcc -e GUI_FitSCLC" in the MatLab command window.

4. A kind request…

If this program was helpful to your paper, please be nice and cite the following work:
"Automated open-source model for reliable charge transport analysis in organic semiconductor diodes" by Nikolaos Felekidis, Armantas Melianas and Martijn Kemerink, [add citation when available]

5. Things to improve

This program has been tested quite extensively, but of course it can always be improved. Things I'm aware of are listed below and will be dealt with when I have time/when there is an urgent need. In case you have requests that you feel might benefit general users, do not hesitate to contact me. Keep in mind though that this is just a fitting program, not a general-purpose drift-diffusion solver or a plotting program. And making the program dual carrier to deal with solar cells and diodes is not an option as the number of parameters will explode, making the thing completely underdetermined.

To improve:

1. add L to filename to allow fitting devices of multiple thicknesses
2. save used filenames?
3. …