**How to use the extended eRDF Analyser: Example with TIF-files from Test\_data**

1. Open RDF\_Analyser\_GUI.m with MATLAB and run the code.
2. **Load the Au calibration file** to calculate the calibration factor *ds*. It is the proportionality between image pixel and reciprocal space for the used measurement setup.
   1. Click ***Load Au SAED TIF***.
   2. The folder “*Test\_data\GST225*” opens. (You can change the default directory in line 185.)
   3. Navigate to “*Test\_data\GST225\00\_gold\_standard\*”.
   4. Choose the SAED pattern “*5484\_970mm\_F20.tif*”. (The other two TIFs are real space images of the gold standard.)
      * The diffraction pattern (DP) opens and the contrast/brightness is manipulated to find the **position of the beam stop** and to mask that area of the beam stop. The masked area is not taken into account when the diffraction profile is calculated.

Notice:

* + - 1. Depending on the **specific TIF format** and the number of layers it contains, the *imread* command in lines 244..256 have to be modified.
      2. **Automated masking of the beam stop is limited to identical beam stops like in the test data**. The procedure works by maximizing the cross-correlation of the contrast/brightness manipulated DP with the datafile MaskShape.txt. The **MaskShape.txt** file (you can open it with Excel or with Matlab command *importdata*) contains a 2028x2048 (resolution of the DP) matrix with zeros (0) and ones (1) as entries. The (1)-entries were designed to mimic the shape of the beam mask and cover it. You can design your own MaskShape.txt to automatically mask the beam stop in your image. **Alternatively, to draw rectangles, ellipses or polygons to mask the desired regions manually**, comment lines 282..333 and uncomment the section **“Add handdrawn masks” (lines 338..488)**.
    - The manipulated DP is also used to **identify circular objects** which are then used as a first guess to **find the center** of the diffraction rings.

Notice:

* + - 1. Depending on the specific form of the DP (e.g. 8 bit/16 bit image), the algorithm might need some adaption of the parameters (lines 498..501).
      2. If successful adaption is not possible, comment the section “Automated center finder” (lines 505..590) and uncomment the section “User input of center” (lines 593..623). You are then asked to input the first guess by yourself, as in the original software.
    - A window opens to ask for three parameters, that are needed for the **optimization of the first guess of the center**. After applying the parameters, the optimization routine (for polycrystalline DPs) from the original software starts.
    - After complete optimization the azimuthal average (azav) and variance (azvar) are plotted and saved as FIG- and TXT-files in the directory of the opened TIF.
    - In the **average intensity plot**, the five most prominent peaks are identified. Their corresponding pixel positions are fitted to the expected reciprocal space vector of Au. The fit is also plotted and saved (as FIG-file) in the same directory as the TIF-file. The **slope corresponds to the calibration factor *ds***. Therefore, *ds* is displayed in the GUI after completion and saved in a separate TXT-file.  
      Notice:
      1. Calibration fit can be adapted in the section “Calibrate peaks to d-spacings” (line 1090 ff.). There, one might want to change the hkl-file (Au\_mean\_std.txt), in case of the usage of a different calibration material. Or different peaks have to be chosen for the fit.
      2. If the checkbox “Load results, if already existent.” is active when the calibration TIF is loaded, the program checks if there is already a corresponding result file (“xyz\_Result\_ds.txt”). If so, the result is immediately loaded into the GUI without a recalculation.

1. **Load the SAED pattern of the “as-deposited” samples**.
   1. Click ***Open SAED TIF(s)*** (with the “Amorphous” radio button active).
   2. The folder “*Test\_data\GST225*” opens. (You can change the default directory in line 1206.)
   3. Navigate to “*Test\_data\GST225\* *01\_GST225\_asd\”.*
   4. **Select all four diffraction TIFs** (“*5519*” to “5523”) at the same time and click open. (The remaining two TIFs are real space images.) In the following, the chosen files are **averaged to a single intensity profile**.
      * Similar to the calibration above, the beam stop is masked automatically as well as the center is found automatically, such that no further user input is needed.

Notice:

* + - 1. Again one can switch from “Automated masking” (lines 1286..1339) of the beam stop to “Add handdrawn masks” (lines 1344..1494) by (un)commenting.
      2. Parameters for automated finding of initial guess of the center: lines 1502..1505.
      3. One can also switch from “Automated center finder” (lines 1510..1593) to “User input of center” (lines 1596..1626).
      4. The above changes also apply if the radio button “Polycrystalline” instead of “Amorphous” is selected in the GUI.
    - A figure with the azimuthally averaged intensity for each DP as well as the corresponding variance is plotted and saved. (“\_AzimAv\_5519\_\_5520\_\_5522\_\_5523\_.fig” & “\_AzimVar\_5519\_\_5520\_\_5522\_\_5523\_.fig”).
    - A TXT-file is saved with the intensity averaged over the selected DPs. (\_sum\_azav\_5519\_\_5520\_\_5522\_\_5523\_.txt)

1. Analogously, **load and average the other SAED patterns** in the folders “*\GST225\02\_GST225\_115C180min*” and “*\GST225\03\_GST225\_150C060min*” subsequently.
2. **Load the averaged 1D profiles that shall be compared** in the terms of S(q) and G(r):
   1. In the GUI click ***Open Folder***.
   2. The folder “\*Test\_data\*” opens. (You can change the default directory in line 2201.)
   3. Choose GST225 as a folder.
      * All TXT-files in the chosen directory that start with “\_sum\_azav” will be displayed to select.
   4. Select the three GST225 files, that were computed in the steps before to compare the different annealing states (“asd”, “115C180min”, “150C060min”), and press ***OK***.
      * The intensity profile are displayed in full in the top graph in the GUI. Below you can see the beginning (middle graph) and the end (bottom graph) of the data range for the loaded profiles.
3. **Enter a start and end data point**, that can be used to extract the structure function S(q) and G(r):
   1. Type “55” in the ***Start*** field and “1400” in the ***End*** field in the GUI.
   2. Click ***Plot selected data***.
4. Go to the **“RDF Plot” tab**, next to the “Diffraction Data” tab (which was active until now) in the upper left corner of the GUI.
5. Enter the **element composition** in the drop-down menus (Ge: 2; Sb: 2; Te: 5).
6. Choose a fit range of 50%.
7. Enter a damping factor (b) for the Lorch damping of 0.1.
8. Click ***Autofit All***.
   * + The fits to the intensity profiles are shown in the upper panel in the GUI.
     + The uncorrected and corrected reduced structure functions are plotted in the middle panel, as well as the uncorrected and corrected pair distribution functions in the lower panel. The correction procedure is described in detail in the publication “Evolution of short-range order of amorphous GeTe upon structural relaxation obtained by TEM diffractometry and RMC methods” (2023).  
       Notice:
       1. The relevant parameters for the correction procedure can be adjusted in lines 3369..3378. In the next steps where S(q) and G(r) are analyzed, the correction degree and other analyzed quantities can be inspected with respect to the different cutoff ranges. Based on that, the parameters (especially numMean and rco) can be adjusted.
       2. A temporary Excel Sheet is created (“*\Extended\_eRDF\_Analyser\results\_temp.xlsx*”) with a number of different formats (including corrected and uncorrected) of the structure function and PDF for export purposes (e.g. for usage in RMCProfile).
       3. The three panels can be exported as a separate figure by clicking ***Export I(q), phi(q), G(r)*** on the lower right side in the GUI.
9. Click ***Analyse S(q)*** above the middle plot in the GUI.
   * + Gaussian fits are done for the first two maxima in S(q) to extract S(q2)/S(q1).
     + Several figures appear showing the fit results for the different correction ranges.
     + Final results (averaged over the set range around rco) are also plotted comparing e.g. S(q2)/S(q1) or the positions of the first two maxima for the three different input files.

Notice:

* + - 1. If the checkbox “Save as figures” (in the GUI above the G(r) plots) is active, all created figures are saved (as FIG, PNG and SVG) in a folder ending with “\_Analyse\_S(q)” in “*\GST225\*”. All files are indicated with time and date.
      2. If the checkbox “Overwrite latest” (in the GUI above the G(r) plots) is active, all figures with the latest time and date are replaced by the newly generated ones.
      3. Completion of the analysis (and saving) is indicted by the output of “S(q) analysis done” in the Matlab console. (Saving might take some time.)
      4. S(q2)/S(q1) is only meaningful in the amorphous phase.

1. Click ***Analyse G(r)*** above the lower plot in the GUI.
   * + Gaussian fits are done for the first seven extrema of G(r) to extract quantities like r2/r1.
     + Several figures appear showing the fit results for the different correction ranges.
     + Final results (averaged over the set range around rco) are also plotted comparing e.g. r2/r1 or the positions of the first seven extrema for the three different input files.

Notice:

* + - 1. If the checkbox “Save as figures” (in the GUI above the G(r) plots) is active, all created figures are saved (as FIG, PNG and SVG) in a folder ending with “\_Analyse\_G(r)” in “*\GST225\*”. All files are indicated with time and date.
      2. If the checkbox “Overwrite latest” (in the GUI above the G(r) plots) is active, all figures with the latest time and date are replaced by the newly generated ones.
      3. Completion of the analysis (and saving) is indicted by the output of “G(r) analysis done” in the Matlab console. (Saving might take some time.)
      4. The two 3D plots showing the relative shifts of the extremum heights and positions might be useful to compare the changes of different input files all at once. The plot is not very useful to compare amorphous with crystalline phases (as in the example presented here).

1. Click ***Compare*** above the lower plot in the GUI to compare to a PDF created by the program [CIF2PDF](https://github.com/CS1910/CIF2PDF).
   1. Navigate to “*\Test\_data\GST225\Crystalline\_PDFs*”, where two examples are saved.
   2. Multiselect both files and open them.
      * Two figures open, showing G(r) of the input files and the crystalline distances computed from crystallographic information files (CIFs).

Notice:

* + - 1. If the checkbox “Save as figures” (in the GUI above the G(r) plots) is active, all created figures are saved (as FIG, PNG and SVG) in a folder ending with “\_Compare\_to\_xyz” in “*\GST225\*”. All files are indicated with time and date.
      2. If the checkbox “Overwrite latest” (in the GUI above the G(r) plots) is active, all figures with the latest time and date are replaced by the newly generated ones.