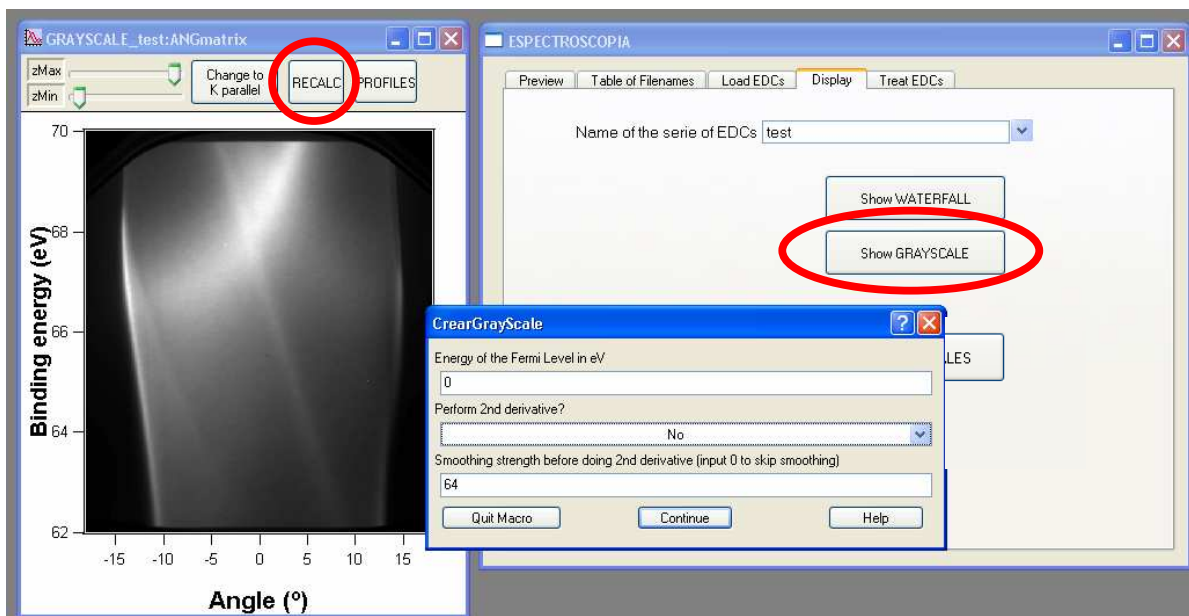


MANUAL for *ESPECTROSCOPIA_v3.ipf* (incomplete)

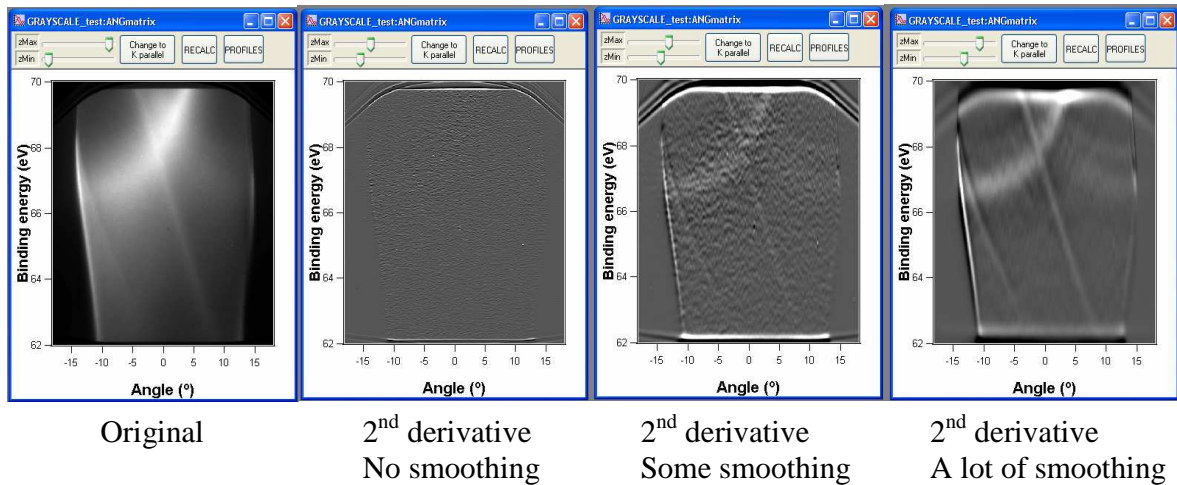
Second derivative in the grayscales:

Every time you press “Show GRAYSCALE” or “RECALC” (marked in red in the image), a window is asking you for three things:



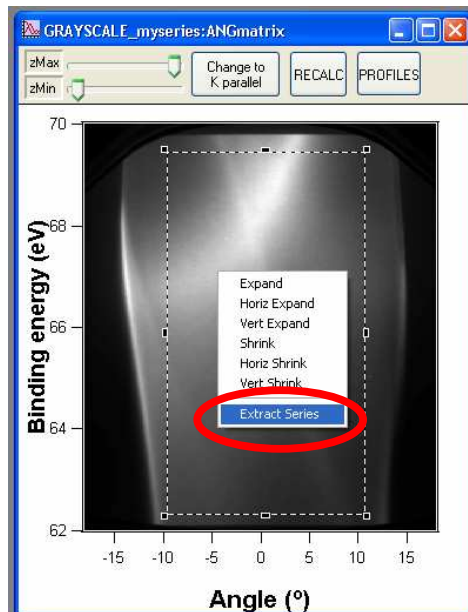
- 1- *Energy of the Fermi Level:* As in previous versions, you can just leave it at 0 if you don't know it. This value can be introduced at anytime by pressing again “RECALC”.
- 2- *Perform 2nd derivative:* Select “Yes” if you want to. By default it says “No”. The second derivative is performed along the energy axis and multiplied by -1, so that you have the same contrast as in the raw image, i.e., more white means more intensity.
- 3- *Smoothing strength before doing 2nd derivative (input 0 to skip smoothing):* This number represents how much the spectra must be smoothed before performing the second derivative (choosing 0 doesn't apply any smoothing). Smoothing is often important if you want to see something in the second derivative, because derivating a noisy image gives nearly anything. Be careful. If you smooth too much, the resulting 2nd derivative image will loose too much resolution in energy. The macro suggests a value by default according to your spectra, but you may play a little bit with this until you get a good compromise between good looking image and not loosing too much information. After getting the second derivative image, you can always come back to the original image by pressing “RECALC” and leaving “No” for the 2nd derivative.

In the following image, you can see the difference between original data, 2nd derivative without smoothing, 2nd derivative with the default smoothing and 2nd derivative with a lot of smoothing. Normally, every time you get the second derivative, it is necessary to play a bit with the contrast using the two slides in the up-left corner of the graph, so that you can see properly your bands.

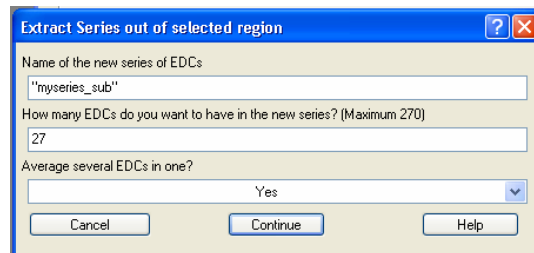


Extracting a region from an existing series:

Select the region of your interest with the marquee and right click. The usual popup menu shows up, where you can now choose “Extract Series”:

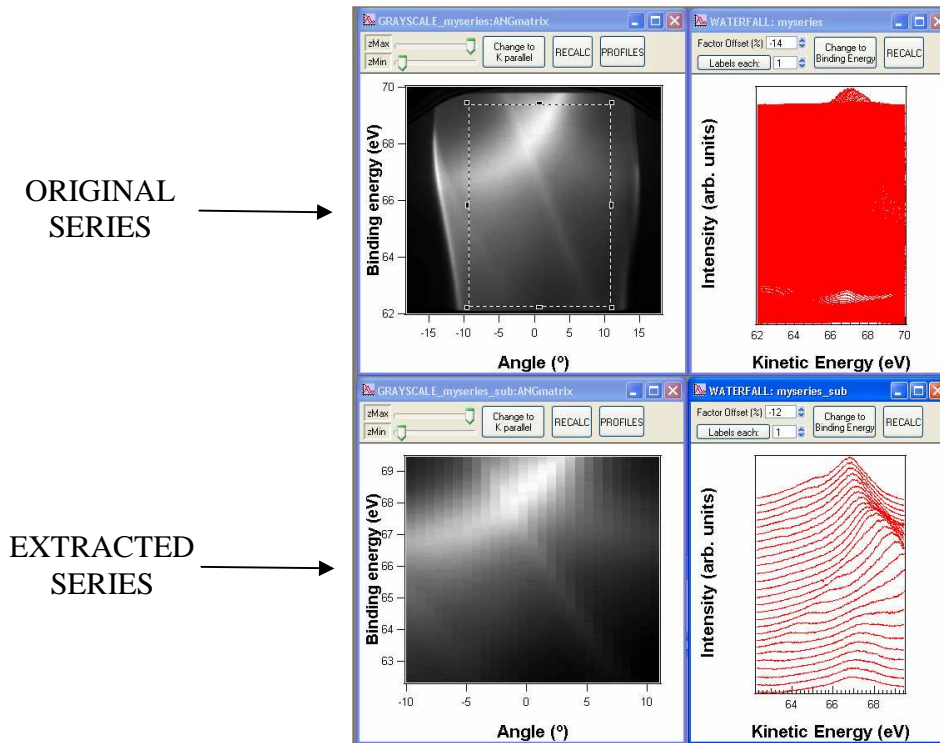


When pressing “Extract Series”, the input window shown below appears:



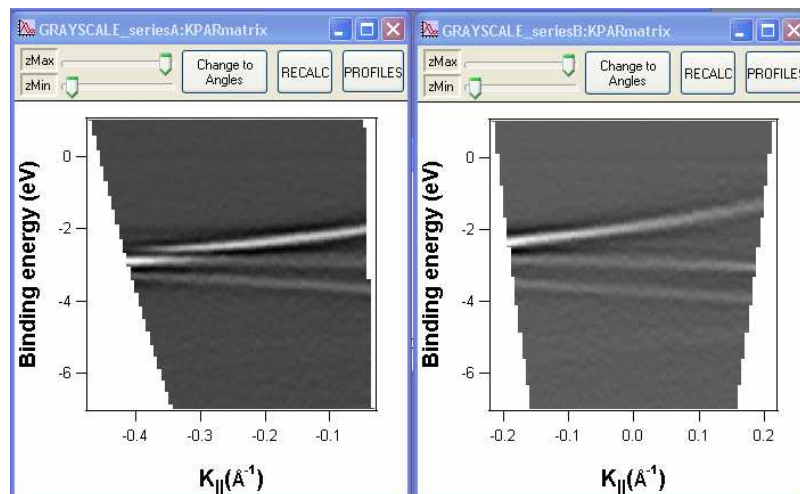
Select the number of EDCs of the new series. For example, if originally you have 270 EDCs, you can reduce to 27, so that one EDC will be extracted from every 10 of the original series. You can choose to average every of these 10 in 1 (saying “Yes”) or just take the first of every 10 (saying “No”).

This operation can only be done in a graph with a Grayscale in Angular mode (not in K parallel), but once you extract it, a new series is created (called “myseries_sub” in the example above) that can be converted to K parallel as usual. Press “Show GRAYSCALE” in the main panel to see the result. Now, the waterfall is much less crowded. Press “Show WATERFALL” to display the waterfall as usual.

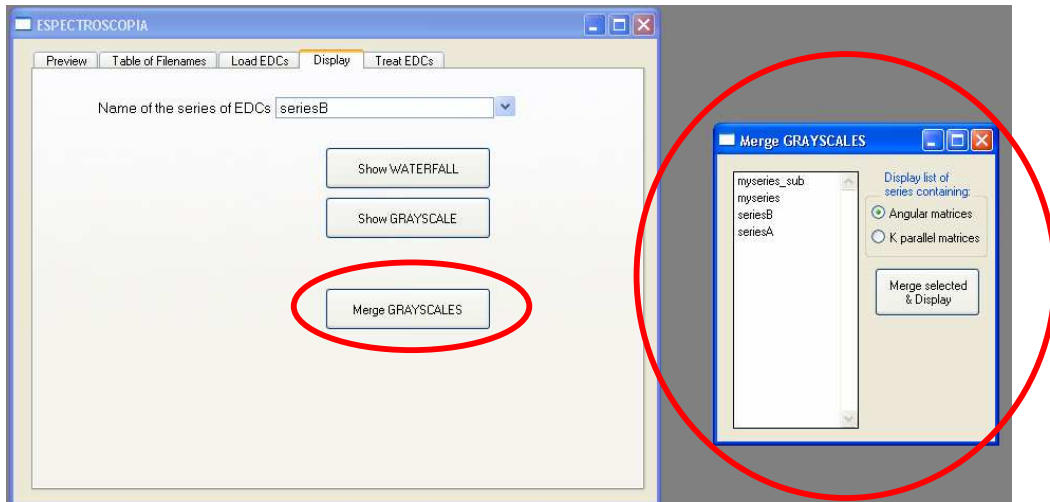


Merging several grayscales in a single one:

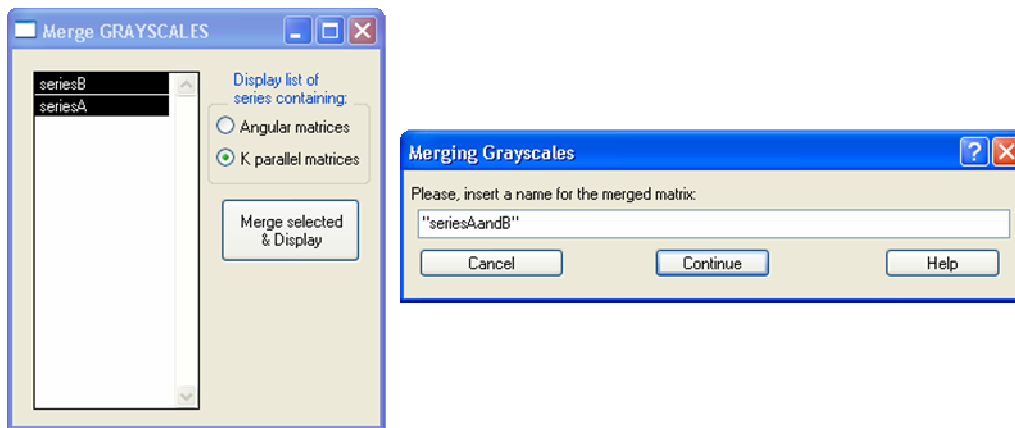
Suppose that you have two series, that are shown below after applying the second derivative and that are represented in K parallel grayscales, as follows:



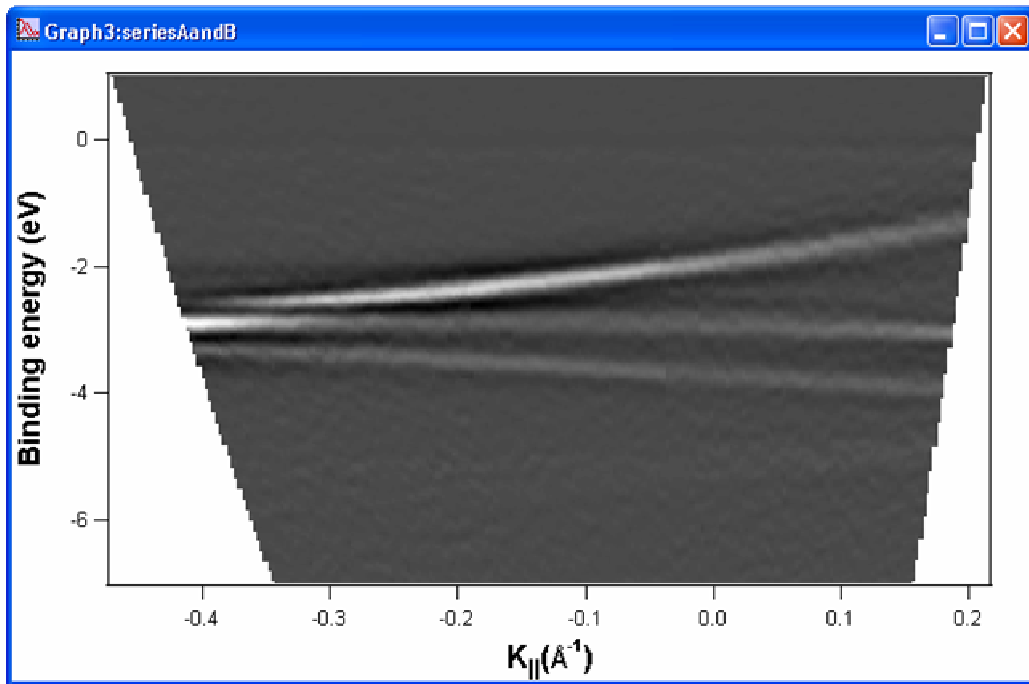
Pressing the button “Merge GRAYSCALES” in the main panel, the panel of the right will appear:



In this panel, selecting “Angular matrices”, the list gives us all the series in which an Angular matrix was created. Selecting “K parallel matrices”, the list refers to all series in which a K parallel matrix was created. Be aware that an Angular matrix is only created within a series if you press “Show GRAYSCALE” in the main panel for that series. The matrix is called “ANGmatrix” and you will find it in the data folder of the corresponding series. Also, the K parallel matrix (called “KPARmatrix”) is only existing if the grayscale is in K parallel mode, like the two series in the example above.



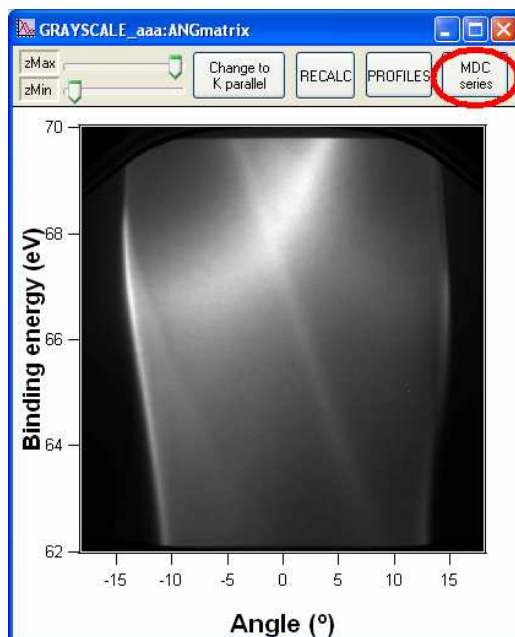
In our case, we want to merge K parallel matrices from the series “seriesA” and “seriesB”. After selecting them from the list, press “Merge selected & Display”. A window will ask you for a name to be given to the merged matrix. This matrix will be saved in the data folder “root:Merged:”. The result can be seen in the following picture:



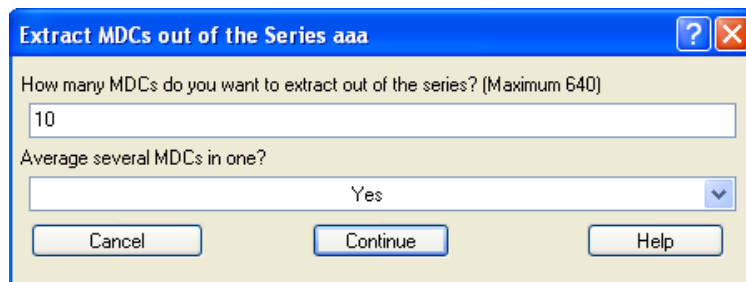
The new matrix is created from the original ones, performing the average in the region where the matrices are intersecting. Of course, the same thing can be done with Angular matrices and in any case, you can choose as many series as you want.

Extracting MDCs from a series of EDCs:

In every grayscale window there is now a new button called “MDC series”.



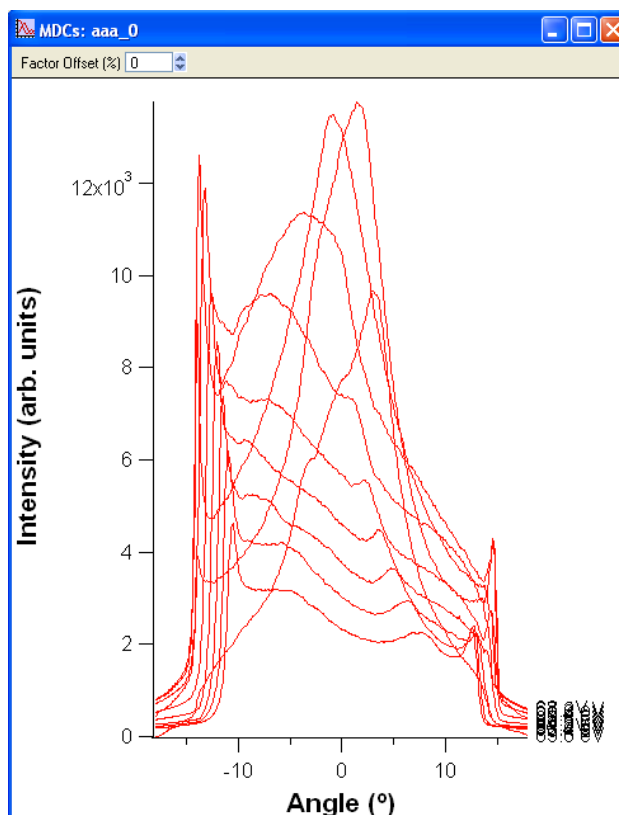
If you press it, the next window will appear:



Select the number of MDCs that you want to extract. For example, if originally your series has 640 MDCs, you can extract only 10 (like in the example above), so that one MDC will be extracted from every 64 of the original series. You can choose to average every of these 64 in 1 (saying "Yes") or just take 10 MDCs equidistant in energy (saying "No"). If you extract all of them (640 in the example), you will normally obtain a very crowded graph, but it is still possible.

When you press "Continue", a new folder will be created called root:MDCs:name_#, where "name" is the name of the original EDC series ("aaa" in the example) and # is an increasing number, because you can extract as many MDC series as you want from a single EDC series.

Also, a new graph will appear with all the MDCs represented:



You can change the “Factor Offset” to avoid the overlapping of the spectra. This Offset can be positive or negative.

