

Analysing RBS data with *Allegria*

The objective of this relatively long example is to show how you can manipulate a spectrum to subtract a background and separate peaks.

1. Download the example:
 - Windows users, download the following file:
<http://www.lps.umontreal.ca/~schiette/Allegria/files/RBSexample.zip> (case sensitive). This file contains the program and a data file used for this example.
 - Linux users, you must have compiled and installed *Allegria*. Then, download the following file: <http://www.lps.umontreal.ca/~schiette/Allegria/files/RBSexample.gz> (data only).
2. Unzip this file in a new directory. (To make sure everything goes well, path name may not contain spaces and letters with accents or other unusual characters.) Linux users must also copy their executable files *SpectrumExtractor*, *Allegria* and *erd2003.exe* to this directory.
3. Fire up *Allegria* from this directory.
4. In the left graph, right-click and select "Load file". Browse down to the "data" directory contained in the new directory you just created, and select the file "STO.dat". This is the RBS spectrum of a Strontium Titanate layer deposited on silicon analysed using a 2 MeV He beam. The peaks, starting from the right, are those of Sr, Ti, Si and O. The Si signal is unusable because it is partially channeled. The purpose of the next 9 steps is to create a separate spectrum for each of the element forming the top layer: Sr, Ti and O.
5. First let subtract the background under the Sr and Ti peaks:
 - a) By left-clicking in the graph area, zoom on the bottom of the Sr and Ti peaks.
 - b) Then, by Ctrl-left-clicking (that is, left-clicking while holding the control key) and dragging, define markers (grey area) on the parts of the spectrum to the left of the Ti peak and to the right of the Sr peak. These markers define the data that will be included in the fit during the following step. If the markers are not properly set, you may clear them by right-clicking in the graph area and selecting "clear markers". Markers may overlap.
 - c) Lets now fit a 2nd order polynomial through the data: right-click on the spectrum name in the legend and select "Fit" from the menu. Select "polynomial", input 2 for the "order" entry field, and check "Interpolate between markers". Click Ok. This will pass a 2nd order polynomial fit in the marked data, which should look like the one on Fig. 1.
 - d) Clear the markers so the next step applies to all data (right-click in the graph area and select "clear markers"). As a matter of fact, operations affect the data of the selected spectrum that are within the grey markers, but will affect the entire selected spectrum if no grey marker is defined.

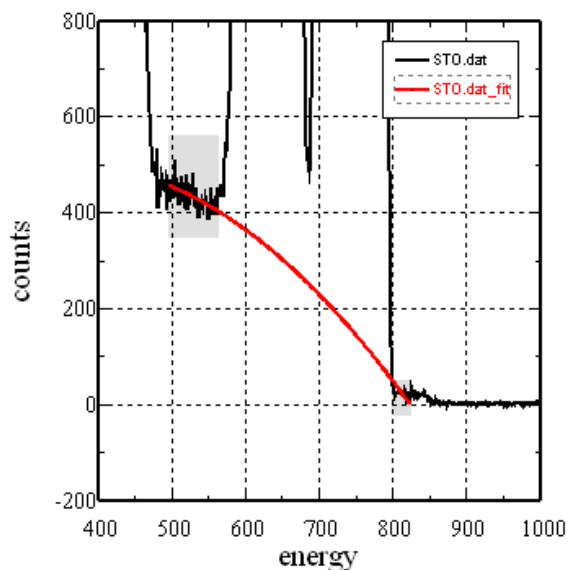


Fig. 1

- e) Subtract this background by right-clicking on the spectrum name in the legend (not the fit), select "Operation" from the menu, select "with data set" then "-" (minus sign), then click the "STO.dat_fit" entry in the list, and then click OK. Ignore the message. The background should now be subtracted. Unzoom by right-clicking in the graph area, and selecting "Unzoom".
 - f) In case you need to restart from this step, save the spectrum as it is by right-clicking on the spectrum name in the legend and selecting "Save". Save under a different file name (for example: " STO_subs.dat") in order to preserve the original data. Delete the background fit dataset by right-clicking on its name in the legend, and selecting "Delete" from the menu.
6. In the following steps, the spectrum will be separated into its different components. Create 2 other copies of the spectrum by right-clicking on the spectrum name and selecting "Copy". Rename and change line colours and width by right-clicking in the legend on each newly copied spectrum name, selecting "Edit" and changing the "Legend" entry and "line options". Use significant name such as "STO.Sr.dat", " STO.Ti.dat " and " STO.O.dat ". Wisely changing the line colour and width will allow you to distinguish superimposed spectra.
 7. By Ctrl-left-clicking and dragging the mouse, define a grey marker that includes the first two peaks. For the spectrum corresponding to O, clear the data included in the grey area by multiplying it by 0: right-click on "STO.O.dat" in the legend and select operation. In the dialog, select "with constant", then "*", and input "0" in the "constant" entry field, then click "Ok". (A shortcut to do this is to hit the "*" key on the keyboard. This will open the Operation dialog with the "*" already selected. You then type "0" which will be inputted in the "constant" entry field, and hit Enter or click "Ok".)
 8. Clear the marker and define a new marker that includes all the data except the Sr peak. Select the Sr spectrum in the legend and multiply by 0.
 9. Clear the marker and define two new grey markers that will include all the data except the second peak, as illustrated in Fig. 2. Select the Ti spectrum and multiply by 0.
 10. Now, lets extract the oxygen peak, identified by an arrow in Fig. 2. For this purpose, we will define a fit under the peak. Clear the grey markers, and zoom on the peak. Right-click below the graph in the X-axis region, and select "Log X axis". You see that the oxygen peak background now looks pretty linear. Define two new grey markers not too far on each side of the oxygen peak. In the legend, right-click on the name of a third (unused) copy of the spectrum and select "Fit". In the dialog, select "Polynomial", input "1" as the order, and click "Ok". One important feature of fitting procedures in *Allegría* is that if you fit a straight line in a semi-log X graph, it will appear as a straight line in this graph and as a " $y = a \log x + b$ " function when you go back to linear axes. The same applies for semi-log Y graphs ($y = b e^{ax}$) and log-log graphs ($y = bx^a$). Tip: if you fit a second order polynomial in a semi-log Y graph, this will correspond to a gaussian function when you go back to a linear Y-axis.
 11. Clear the grey markers, right-click on the O spectrum legend entry and select "Operation" from

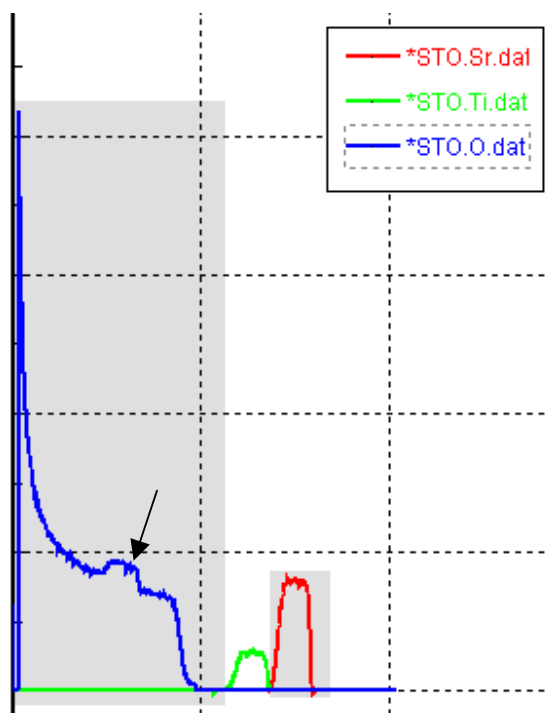


Fig. 2

the menu. In the dialog, select "with dataset", then "-" (minus), and the entry in the dataset list that corresponds to the fit (STO.O.dat_fit). Click "Ok". Ignore the message. You may delete the dataset corresponding to the fit by right-clicking on its name and selecting "Delete" from the menu.

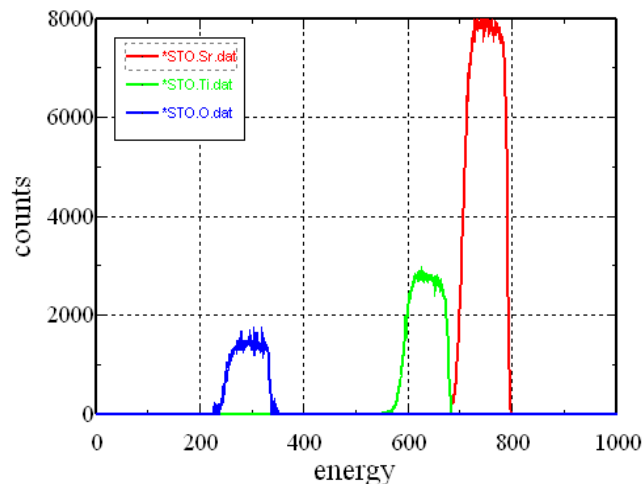


Fig. 3

12. Unzoom, and define two grey markers that include all the data except the background-subtracted oxygen peak. Select the O spectrum and multiply by 0.
13. You now have the three spectrum components separated as in Fig. 3. You can move the legend out of the way by changing its position: right-click in the graph area and select "Edit legend". (Remember that at this point, no data were saved so they all live only in the computer's memory. If you delete them or quit *Allegria*, they are lost and you have to start over.) One side effect of the manipulations we did is that all operations were made considering that the data are floating points. However, *erd2003* (the program that makes the spectrum to depth profile conversion) only accepts integer. Passing spectra containing fractional counts values to this program will generate a Fortran error. Thus you must save manually all spectra by sequentially applying the "Save selected energy spectrum as integer" command from the "File" menu to each of them. Don't use the "Save" command from the right-click menu, which would save fractional count spectra. All spectra must be saved in the same directory as the original spectrum.
14. Now the depth profile conversion: open the "Experimental Parameters" dialog by selecting "Conversion > Experimental parameters" from the menu.
15. Click the "Select Dir" button and browse down to the directory where the spectra extracted in the previous steps are stored. Click "Ok".
16. Click on the "Element" tab. For each of the three elements, click on its tab and, if it is not already entered, type the corresponding spectrum filename (bottom right entry field), or press the "... " button to select from a file dialog.
17. Click "Ok" to close the "Experimental Parameters" dialog. Click "Ok" to the message "Beam parameters...".
18. Start the conversion: select "Conversion > Go" from the menu. *Allegria* first loads the saved spectra to make sure they are available, and ask the user if the data already present on the graph can be cleared; answer "yes", and answer "Ok" to the "Beam parameters..." message. If every thing goes well, you should see (in a DOS window for Windows users, in the console for Linux users) this message: "Iteration 1 starting", than 2, then 3. The resulting profiles (after 3 iterations) will show up in the "Depth profiles" window of *Allegria*.
19. You may zoom the profiles by clicking in the graph region and dragging the mouse over the profiles. To unzoom, right-click and select "Unzoom". Depth profiles data can be saved in a single, multi-column file by selecting "File > Write Depth Profiles in a single file" from the menu. This is useful for importing the data to other graph plotting programs. However, *Allegria* cannot read back this file format.