INTERFERE and MERGE - using Microsoft Excel to choose parameters for LAD data

Alex C. Hannon
ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, UK.

Abstract

The ATLAS suite enables a user to correct and reduce neutron diffraction data for a non-crystalline sample obtained on the LAD diffractometer. In the ATLAS suite the program INTERFERE is used to re-normalise the data and subtract the self scattering, and then the program MERGE is used to combine the data from different angles to produce a single merged result. In practice a large number of iterations of the two programs is required in order to choose suitable parameters to give an acceptable result. An alternative method for choosing the parameters, based upon Microsoft Excel, is described here. When using this method, the parameters feed automatically into the calculation so that their effect is immediately apparent.

1. Introduction

When using the ATLAS suite [1,2] to analyse LAD [3] data, a large number of iterations may be needed to satisfactorily complete the INTERFERE and MERGE processes. When performing these iterations, the effect of the choice made for a particular parameter may not be immediately apparent. This document describes an alternative method for choosing the parameters, based upon Microsoft Excel. When using this method, if a parameter is changed then the new value is automatically fed into the calculation without having to re-run any programs, and its effect is seen straight away. The method may also be useful as a 'tutorial' to show the effects of the various parameters.

2. INTERFERE and MERGE in the ATLAS suite

It is assumed here that the ATLAS suite has been used to produce a .DCS file which contains the corrected total scattering $I(Q)$ for the usual 14 LAD detector groups. It is also assumed that the ATLAS suite has been used to calculate a .SLF file which contains the self scattering $I^S(Q)$ for each detector group. The INTERFERE process involves subtracting the self scattering from the total scattering for each group, to yield the distinct scattering

$$i_i(Q) = \alpha_i I_i(Q) - I_i^S(Q), \quad (1)$$

where $i_i(Q)$, $I_i(Q)$ and $I_i^S(Q)$ are respectively the distinct, total and self scattering for the i^{th} detector group. α_i is the re-normalising factor for the i^{th} group. Ideally all re-normalising factors should be equal to one, but in practice it is necessary to multiply the total scattering by a factor a little different from one in order to yield a result from eqn. (1) which oscillates about zero. A slightly different value will be needed for α_i for each detector group, but the values should not differ markedly from one. In the ATLAS suite the program INTERFERE is used to apply eqn. (1) to the .DCS and .SLF files, and put the distinct scattering for each detector group into a .INT file.

In the ATLAS suite the MERGE program is used next to combine the distinct scattering for all of the groups into one composite curve (a .SOQ file), covering the widest Q-range possible. For each group the user specifies the reliable Q-range by giving Q_{min} and Q_{max}.

3. Getting the data into the Excel workbook

Once the ATLAS suite has been used to produce the .DCS and .SLF files for the sample, the data can be put into files suitable for input to the Excel workbook by typing @g_f:PC in GENIE [4]. This creates output files named DCS12345.PC and SLF12345.PC. These are ASCII files and should be copied to the hard disk of the PC. At present the data are binned with a maximum Q of 40Å^{-1} and with a Q-spacing of 0.1Å^{-1}.

An example Excel workbook INTMER.XLS is available. This may be obtained via the World Wide Web by connecting to the ISIS Disordered Materials Home Page (http://isis.rl.ac.uk/disordered) and following the links to the Software Downloads page. The file is also available on the ISIS PC network on the "Babylon" area as \ACH\Intmer\INTMER.XLS. Furthermore the file may be obtained direct from the author, but please note that its size is nearly 3 Megabytes, which is too big for a floppy disc.

Copy the file INTMER.XLS to your PC and rename it to a suitable name e.g. SAMPLE1.XLS. In order to get the data into the Excel workbook on the PC, adopt the following procedure:

1. Use the ATLAS suite to produce the .DCS and .SLF files.
2. In GENIE type @g_f:PC to produce the files DCS12345.PC and SLF12345.PC.
3. Copy the two files to the PC.
4. Start Excel.
5. Click the File menu and then Open.
6. Open the DCS12345.PC file. The data will be read in as a worksheet (take the defaults offered at each stage of the "Text Import Wizard").
7. Once the file has been imported, click the "select all" button (this is the unmarked button to the left of "A" and above "1").
8. Copy the data to the clipboard.
9. Close the file DCS12345.PC. (Make sure that the data are not lost from the clipoard).
10. Open the workbook SAMPLE1.XLS.
11. Go to the worksheet named DCS and position the cursor at cell A1.
12. Paste the data into the worksheet.

Then repeat the above procedure (steps 5 to 12) to get the data from the file SLF12345.PC into the worksheet named SLF. Figure 1 shows an example of the SLF worksheet for a tellurite glass [5].

4. The contents of the Excel workbook

Once the data are in the workbook, it can be used to choose optimum values for the re-normalising factors α_i and Q-limits for each detector group. The workbook also allows for the possibility that it may be necessary to add a straight line to each $i_i(Q)$ due to an imperfect result having been obtained from the ATLAS suite;

$$i_i(Q) = \alpha_i I_i(Q) - I_i^S(Q) + A_i Q + B_i, \quad (2)$$

where A_i is the gradient of the linear correction and B_i is its intercept. It is necessary to use non-zero values for A_i and B_i when the $i_i(Q)$ calculated according to eqn (1) is not horizontal over a range in Q in which it might be expected to be horizontal. Caution should be exercised in using this linear correction because a necessity for non-zero values of A_i and B_i may indicate that the absorption correction (calculated by CORAL) has not been performed correctly due to the use of an incorrect numerical value (such as effective number density, radius or absorption cross-section). Possible reasons why the linear correction may be necessary include the presence of a small amount of hydrogen in the sample (usually as -OH or H_2O) or the effect of a low energy nuclear resonance for one of the isotopes in the sample.

The first two worksheets of the workbook contain the data from the ATLAS suite. These worksheets are named DCS and SLF, and they contain the data from the LAD12345.DCS and LAD12345.SLF files respectively. The SLF worksheet shows a plot of the self scattering $I_i^S(Q)$ for each of the seven LAD detector angles (see Figure 1). In the example workbook INTMER.XLS the maximum y-value of all of the plots is set to be suitable for a sample for which the self scattering level ($\sigma_{scatt}/4\pi$) is about 0.33 barns atom^{-1} steradian^{-1}. For a sample with a significantly different value for σ_{scatt} it will be necessary to modify the y-limits of all of the plots in the workbook.

The next seven worksheets show data for each of the seven LAD detector angles (5°, 10°, 20°, 35°, 60°, 90° and 150°). Each of these worksheets has two plots of the data and also contains the relevant values of α_i, A_i and B_i. The first plot shows $I_i^S(Q)$ and the two $\alpha_i I_i(Q) + A_i Q + B_i$ (for the two sides of the instrument), whilst the second plot shows the two $i_i(Q)$ together with current merged $i(Q)$. Both of these plots can be used as a guide to set the value of α_i (and A_i and B_i if necessary). The second plot is also useful for choosing the reliable Q-range (Q_{min} and Q_{max}) for each detector group. The relevant Q-limits are shown on these worksheets for reference, but they may not be set at this point. Figure 2 shows as an example the 150° worksheet for a tellurite glass [5].

The seven worksheets for the individual LAD detector angles are followed by a worksheet named QLIM. This worksheet is used to set the values of Q_{min} and Q_{max} for each detector group and it shows plots of the current merged $i(Q)$. The worksheet also repeats the values for α_i, A_i and B_i for

convenience, but note that the values for these parameters cannot be set on this worksheet. Figure 3 shows as an example the QLIM worksheet for a tellurite glass [5].

The QLIM worksheet is followed by three worksheets named ALF, LIN and LIM. These three worksheets contain copies of the final parameters in a format suitable for producing output files for use in the ATLAS suite. On each of these worksheets the required data is surrounded by a border. Probably the easiest way to get the numbers out of Excel is to select the required area and then copy and paste it to some other application, such as Microsoft Notepad, from which they can more easily be saved as a text file (for use by ATLAS on a VMS computer).

The three final worksheets (DCS2, INT and MERGE) are used for performing the calculations and should not normally be modified at all.

5. Suggested procedure for using the Excel workbook

Once the data have been inserted in the workbook, using the method described above in section 3, the following procedure is suggested for setting the parameters:

1. Start with the highest angle data.
2. Choose the re-normalising factors α_i to make each $\alpha_i I_i(Q)$ oscillate about $I_i^S(Q)$.
3. If necessary set the straight line gradient A_i and intercept B_i so that $i_i(Q)$ oscillates about zero over the full Q-range likely to be used (perhaps 15 to 40 Å^{-1} for LAD 150° detectors - see Figure 3).
4. Choose the Q-limits. For the highest angle data (150° on LAD) the value of Q_{min} is usually somewhere between 10 and 15Å^{-1} - below this value the highest angle data become inconsistent with lower angle data due primarily to the Placzek effect (see figure 2 for example). The value of Q_{max} should be chosen to be the highest Q at which information can be discerned.
5. The above procedure should then be repeated for the next highest angle (90° on LAD), and so on down to the lowest angle.

It is generally advisable to choose the Q-limits to be where the slope is small (e.g. at the top of a peak or at the bottom of a trough). This approach reduces the risk of obtaining significant steps in the final merged $i(Q)$ at any of the Q-limits. The only limits where this consideration is not important are the very highest Q_{max} and the very lowest Q_{min}. Note that if Q_{min} for a particular group is set higher than Q_{max} then this has the effect of completely omitting that group from the final merged $i(Q)$.

6. Using the parameters with the ATLAS suite

The weighting scheme used by the Excel workbook to merge the data simply involves ones and zeros. This is to be contrasted with the MERGE program in the ATLAS suite which uses a more sophisticated scheme based upon the incident flux corresponding to each data point (as determined by the vanadium run). For this reason it is recommended that, once the Excel workbook has been used to obtain a satisfactory set of parameters (α_i, A_i, B_i and the Q-limits), the final analysis is done using the ATLAS suite. The parameter values can be entered into the calculations performed by the ATLAS suite

by putting them into files named .ALF, .LIN and .LIM respectively. The appendix shows typical examples of these parameter files. The ATLAS program area g_f contains template files, named g_f:TEMPLATE.ALF for example, which may be used as a basis for producing parameter files for use with the ATLAS programs.

The .ALF file contains the renormalising factors α_i and is used by the ATLAS program INTERFERE to perform the operation defined by Equation (1). The output file from INTERFERE has extension .INT.

The .LIN file contains the linear correction parameters A_i and B_i. If a linear correction is to be performed then this may be done in GENIE by running the program @g_f:LINT and this should be done after running INTERFERE and before running MERGE. Note that this program is not described in the ATLAS manual. The input to this program is a file with extension .INT, whereas the output has extension .LNT. If a linear correction is made to the data then care should be taken when running MERGE to use the .LNT file, rather than the .INT file.

The .LIM file contains the minimum and maximum values of Q for each of the groups to be included when running MERGE.

After running the ATLAS programs with the parameters determined using the Excel workbook it is advisable to check carefully whether it is necessary to fine-tune some of the parameters.

7. Additional points

The software (both PC.COM and INTMER.XLS) has been set up so that the data are treated with a maximum Q of 40Å^{-1} and a Q-spacing of 0.1Å^{-1}. In order to treat the data with a different set of Q-values it is necessary to do two things:

1. Copy the file PC.COM from g_f to your own area and change the two lines containing a REBIN command (reb w1 0 (0.1) 40) to have the required maximum Q and Q-spacing.
2. Modify the Excel workbook to cover the required Q-range. If the number of points is to be increased then this involves extending downwards the defined cells on the worksheets DCS2, INT and MERGE. It is also necessary to extend the range of data plotted on each worksheet.

The Excel workbook INTMER.XLS has been set up with protection so that it is not immediately possible to change anything other than the values for α_i, A_i, B_i and the Q-limits, and these may only be changed on the correct worksheet. This protection can be turned off from the Tools menu in Excel (no password is necessary).

Acknowledgement

Thanks are due to Norimasa Umesaki for an invitation to visit Osaka National Research Institute (ONRI) where the software described here was conceived and written.

References

[1] A.K.Soper, W.S.Howells and A.C.Hannon, Rutherford Appleton Laboratory Report RAL-89-046 (1989).

[2] A.C.Hannon, W.S.Howells and A.K.Soper, IOP Conf. Series 107(1990)193.

[3] W.S.Howells, A.K.Soper and A.C.Hannon, in: Rutherford Appleton Laboratory Report RAL-90-041 (1990) page 24.

[4] W.I.F.David, M.W.Johnson, K.J.Knowles, C.M.Moreton-Smith, G.D.Crosbie, E.P.Campbell, S.P.Graham and J.S.Lyall, Rutherford Appleton Laboratory Report RAL-86-102 (1986).

[5] A.C.Hannon, N.Umesaki and M.Tatsumisago, to be published.

Appendix - example ATLAS Parameter Files

This appendix shows typical example .ALF, .LIN and .LIM parameter files for LAD.

LAD12345.ALF

```
14
1    1
2    1
3    1.05
4    1.04
5    1.13
6    1.18
7    1.085
8    1.12
9    1.057
10   1.075
11   1.12
12   1.13
13   1.036
14   1.04
```

The first line gives the number of groups. The value of the renormalising constant α_i is then given for each group.

LAD12345.LIN

```
14
1    0
2    0
3    0
4    0
5    0
6    0
7    1    -0.002     0.01
8    1    -0.002     0.01
9    1    -0.0013    0.017
10   1    -0.0013    0.017
11   1    -0.0007    0.011
12   1    -0.0003    0.004
13   1    -7.5E-05   0
14   1    -7.5E-05   0
```

The first line gives the number of groups. For each group a flag (1 or 0) then indicates whether the linear correction is to be performed. The gradient A_i and intercept B_i are given for each of the groups to be corrected.

LAD12345.LIM

```
14
1    0
2    0
3    1    0.32       4.18
4    1    0.32       3.3
5    1    1.74       8.88
6    1    1.42       8.74
7    1    1.38       16.70
8    1    3.88       16.74
9    1    3.88       21.22
10   1    6.04       21.22
11   1    6.12       26.34
12   1    3.92       24.58
13   1    14.38      50
14   1    14.38      50
```

The first line gives the number of groups. For each group a flag (1 or 0) then indicates whether the group is to be included in the merging process. The minimum and maximum values of Q are given for each of the groups to be included.

Figure Captions

1. The SLF worksheet from the workbook for a tellurite glass with 10 mol% K_2O [5].
2. The worksheet for the LAD 150° detectors for a tellurite glass with 10 mol% K_2O [5].
3. The QLIM worksheet for a tellurite glass with 10 mol% K_2O [5].