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Use of the IBA DataFurnace

C. Jeynes
University of Surrey Ion Beam Centre
U.K.

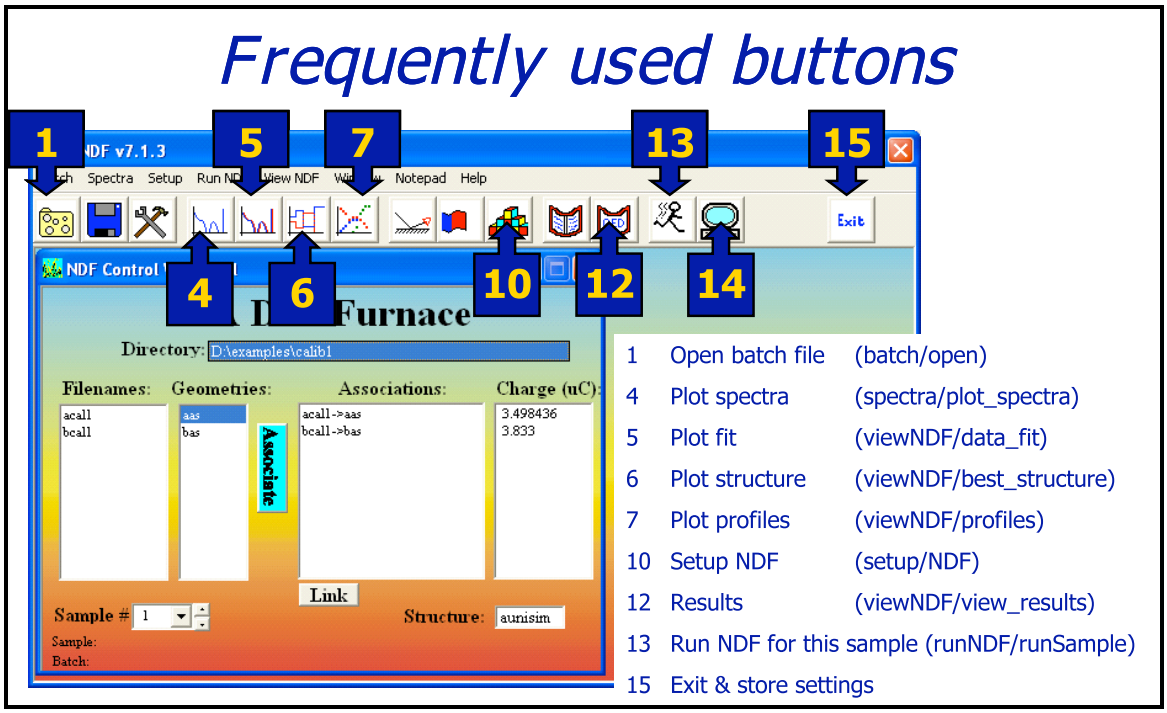
IBA techniques: Practical Session

Use of the IBA DataFurnace

Introduction

The DataFurnace can be used for all particle scattering data (ie. RBS, EBS, ERD, NRA but *not* PIXE at present) to obtain depth profiles, and is a sophisticated code. Some acquaintance with it is also useful to all who may make use of the IBC's depth profiling facilities.

We start with an introduction to the windows:



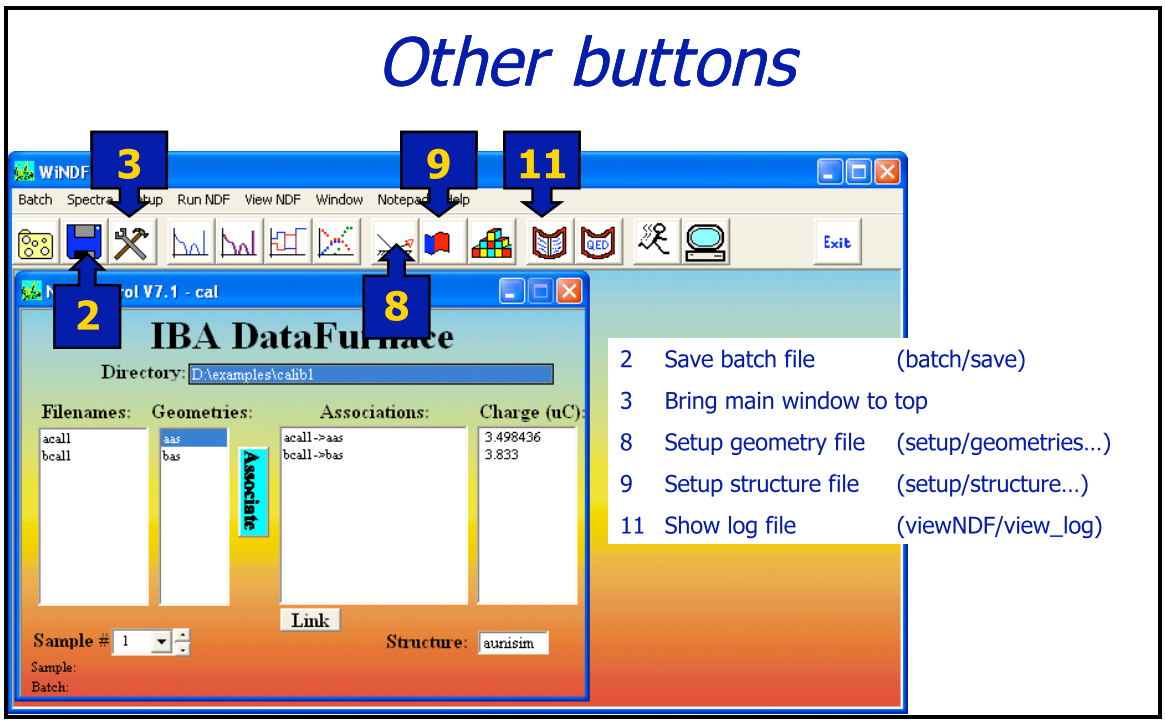
The buttons are accelerators. Most of the functions can be accessed through the menu (these are indicated in the box). Note also that keyboard accelerators are indicated on their menu commands.

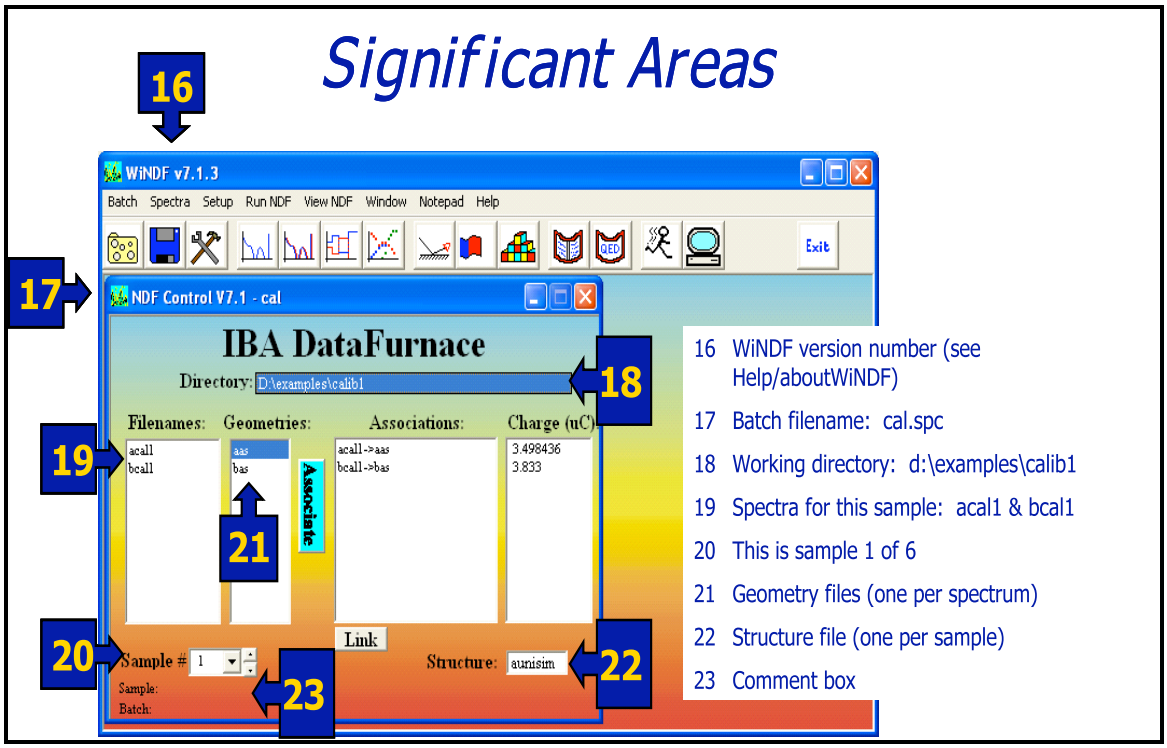
A "sample" (#20) is defined by one or more spectra (#19). Typically we have two spectra collected simultaneously from two detectors in the chamber (see "Simultaneously collected spectra": this option, #27, can be used if the relative charges are known well enough).

The structure file (#22) restricts the state space which is searched for a solution.

The geometry file (#21) determines the geometry *associated* (#28) with each spectrum.

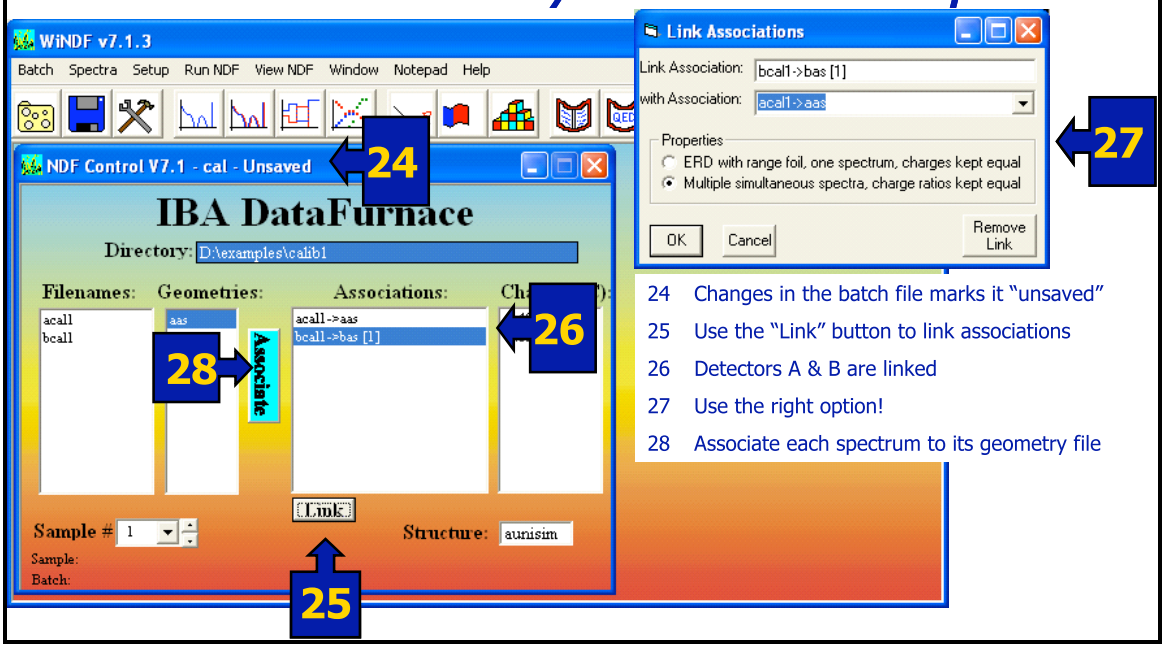
The batch (#17) is a set of samples. These will often be similar samples with the same geometry and structure files.





You can either open a batch file directly with "Open Batch" (#1) or switch the directory by clicking on the directory window (#18). If there is no batch file in a directory you have to start somewhere. All related spectra are gathered together into one directory. NDF only works inside a directory: there are very many output files and we use the directory structure to organise them together.

Simultaneously collected spectra



24 Changes in the batch file marks it "unsaved"

25 Use the "Link" button to link associations

26 Detectors A & B are linked

27 Use the right option!

28 Associate each spectrum to its geometry file

Exercise 1: Calibrations

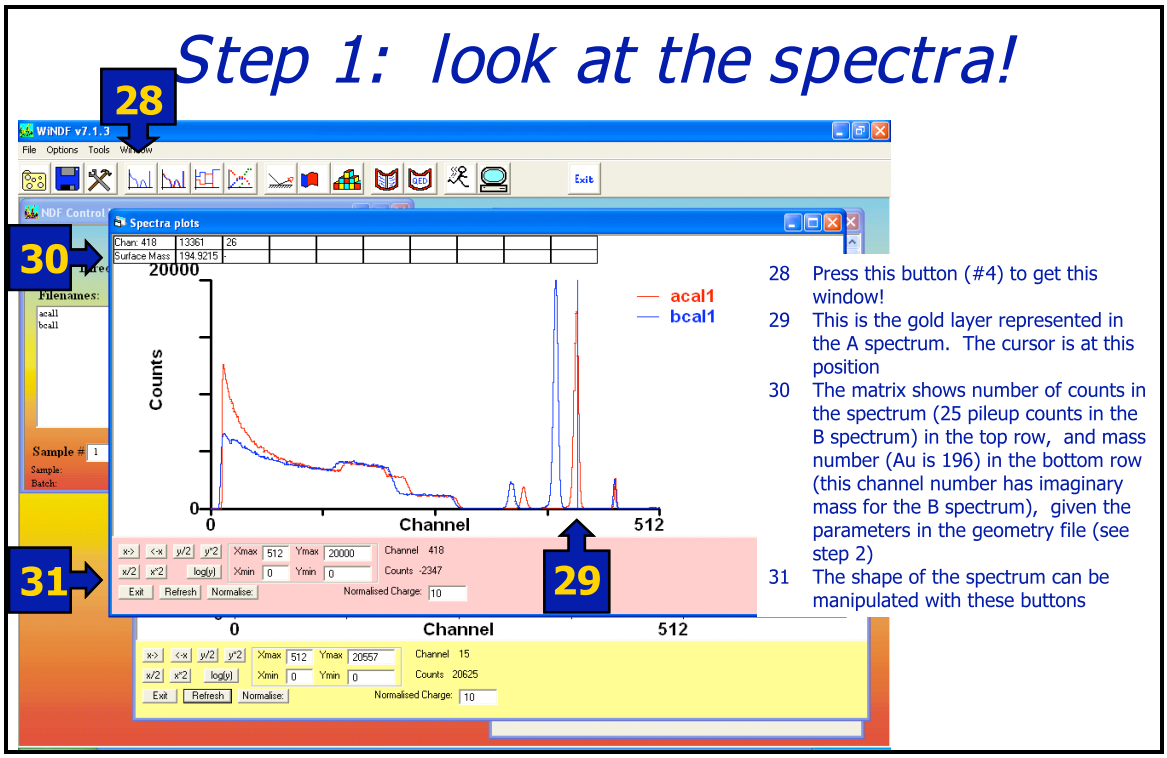
Open /examples/calib1. This is Example 1 on the website (www.ee.surrey.ac.uk/ibc/ndf)

The calibration sample is Au/Ni/SiO_2/Si substrate, where the metal films are very thin (~1.5nm) and the oxide film is ~150nm thick. This sample has been discussed extensively in Jeynes *et al*, NIM **B137** (1998) 1229.

We can use the 4 elemental edges to do a linear regression to obtain the gain g (in keV/channel) and offset o (in keV) of the electronics calibration:

$$E = g.C + o$$

where E is the energy of the scattered particle and C is the channel number in which the elemental edge appears. In principle, the detector does not register the energy E but a slightly lower energy due to energy loss through the detector dead layer and other effects (this is discussed extensively in the NIM B137 reference) but we usually ignore this "pulse height defect" effect. Actually, the fact that the offset o is non-zero is due to the pulse height defect.

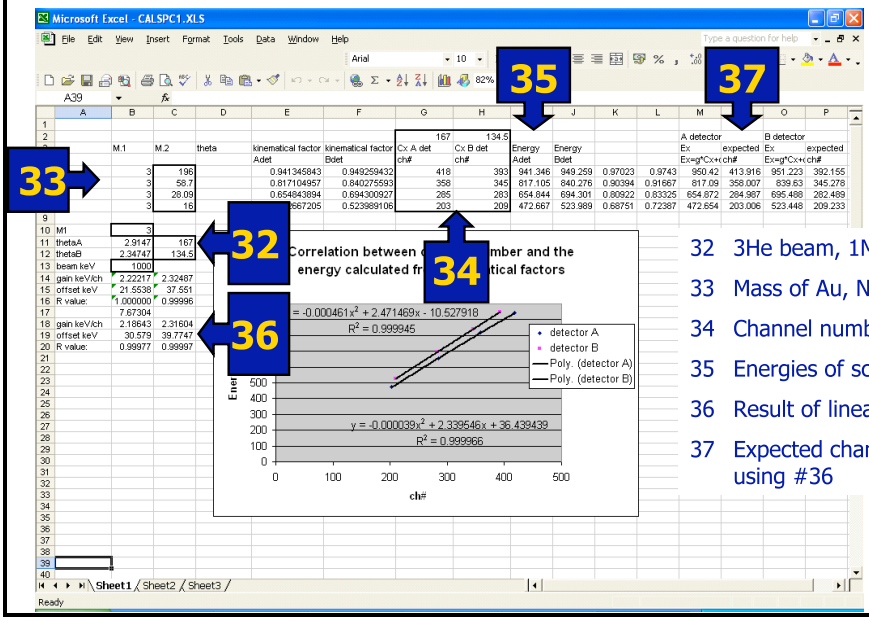


In the example the calibration is already done, but we will show the working.

Look at the spectra (Step 1). The elemental edges are at channel numbers 417, 358, 281, 199 (Au, Ni, Si, O edges respectively) for the spectrum from the A detector (red data), and 394, 343, 278, 204 for the B detector.

We have constructed a spreadsheet (calspc1.xls) to do the linear regression, and the values of gain and offset are entered in the *geometry file* (#21).

Linear regression



32 3He beam, 1MeV, scattering angles

33 Mass of Au, Ni, Si, O

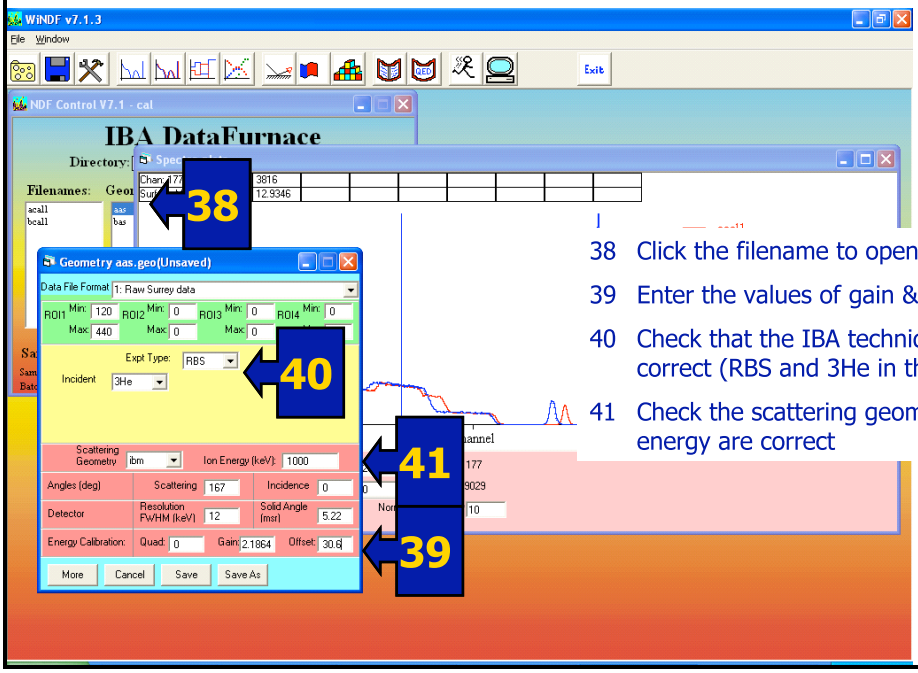
34 Channel numbers of elemental edges

35 Energies of scattered particles

36 Result of linear correlation

37 Expected channel numbers of edges using #36

Geometry File



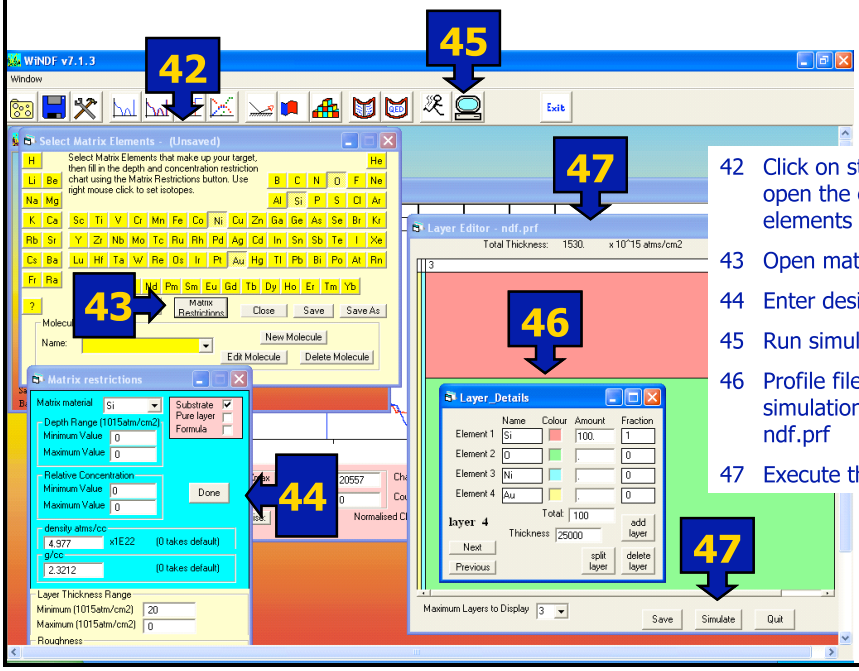
38 Click the filename to open the editor

39 Enter the values of gain & offset

40 Check that the IBA technique and beam are correct (RBS and 3He in this case)

41 Check the scattering geometry and beam energy are correct

Simulating the spectrum



42 Click on structure file name (#22) to open the editor; select required elements (Au, Ni, Si, O)

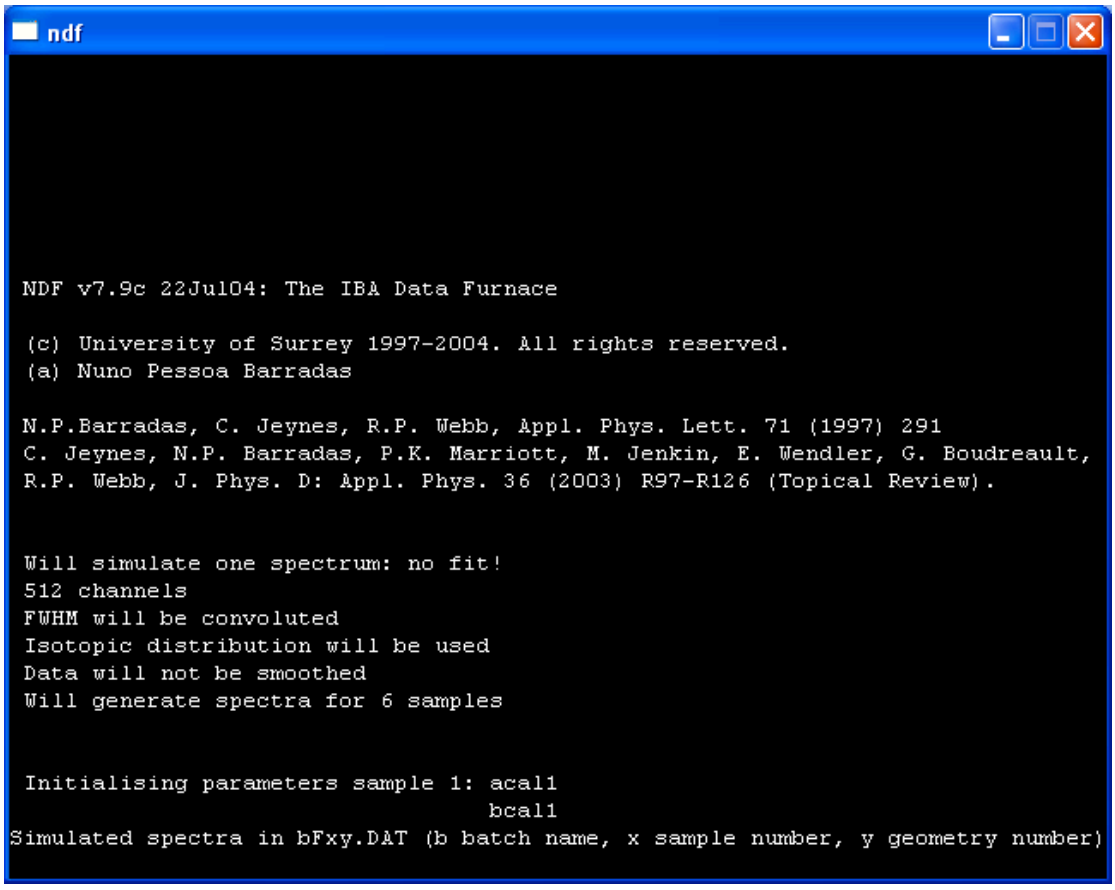
43 Open matrix restrictions window

44 Enter desired restrictions

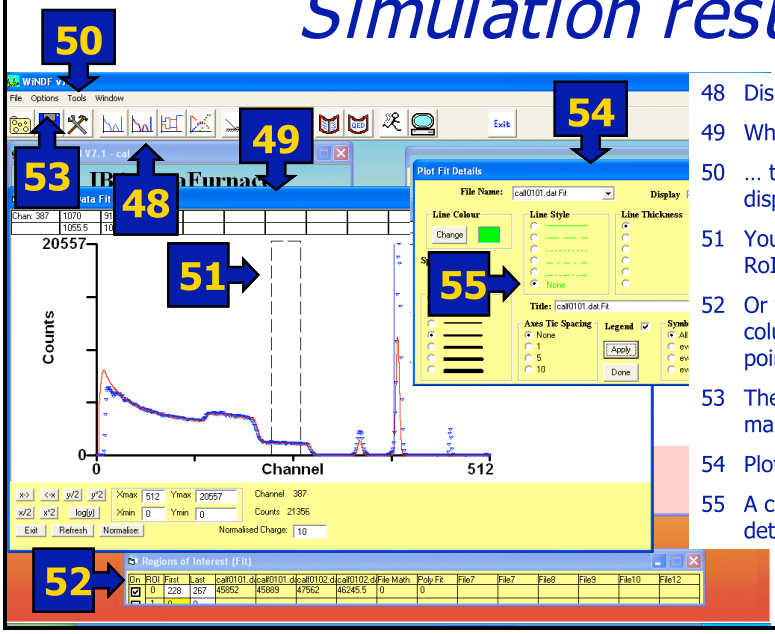
45 Run simulation

46 Profile file editor (ndf.prf). The simulation is of the structure given by ndf.prf

47 Execute the simulation



Simulation result



48 Display the result of the simulation

49 When the fit window is on top: …

50 … the menu changes. The RoI is displayed from here

51 You can click on the window to fix the RoI

52 Or you can click in the "First" and "Last" columns to change the typing entry point

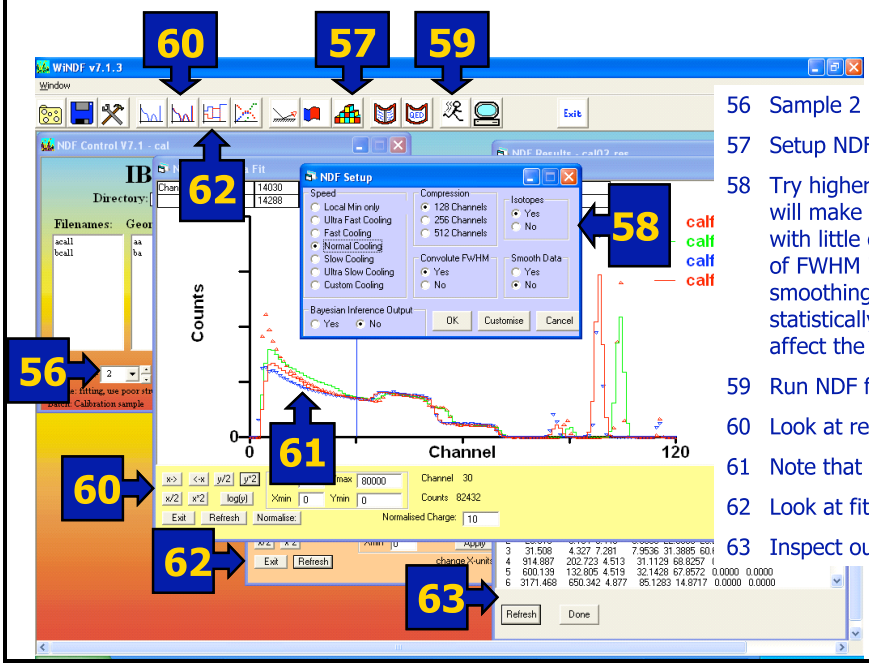
53 The display of the fit window can be manipulated using Options/Plot

54 Plot details window

55 A convenient way to make the A detector spectrum invisible

Using the simulator we check that the gain and offset , and the solid angle, are reasonable. For the solid angle we check that the Si signal from the SiO2 is the right height using the RoI window.

Fitting with NDF: 1



56 Sample 2

57 Setup NDF

58 Try higher speeds first, compression will make NDF run faster frequently with little or no penalty, convolution of FWHM is critical to good fitting, smoothing data is not valid statistically, isotopes will significantly affect the Ni signal

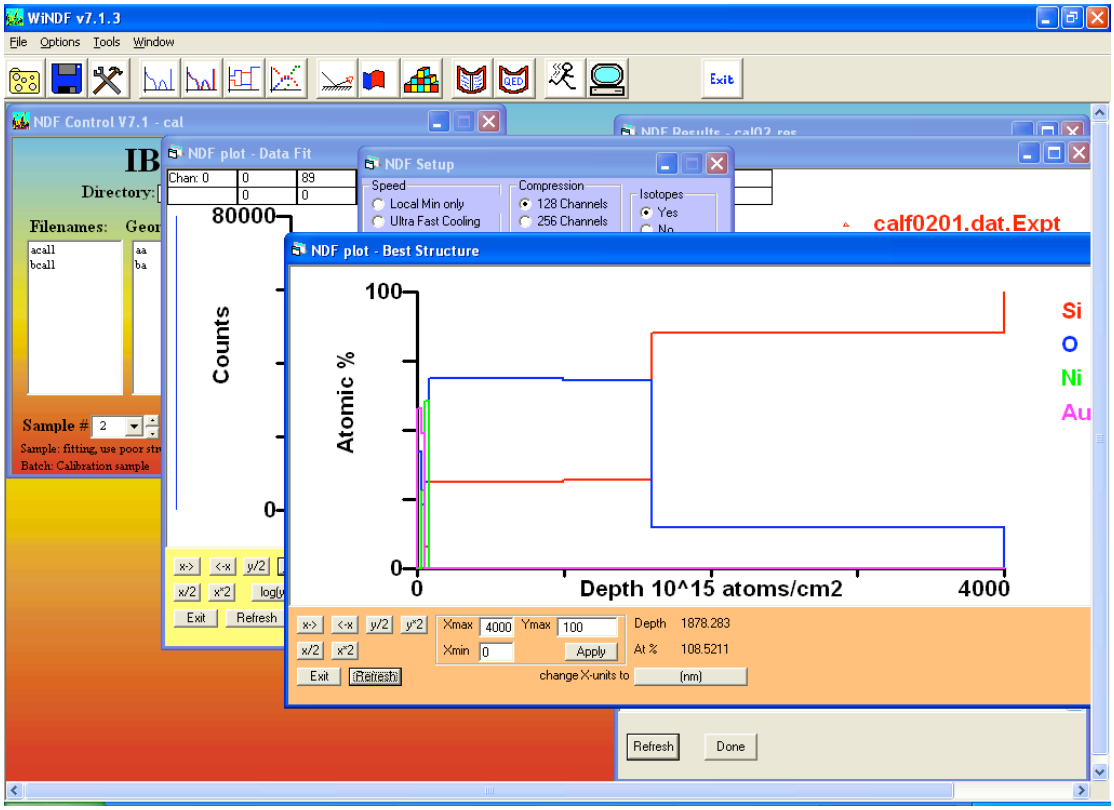
59 Run NDF for this sample

60 Look at resulting fit

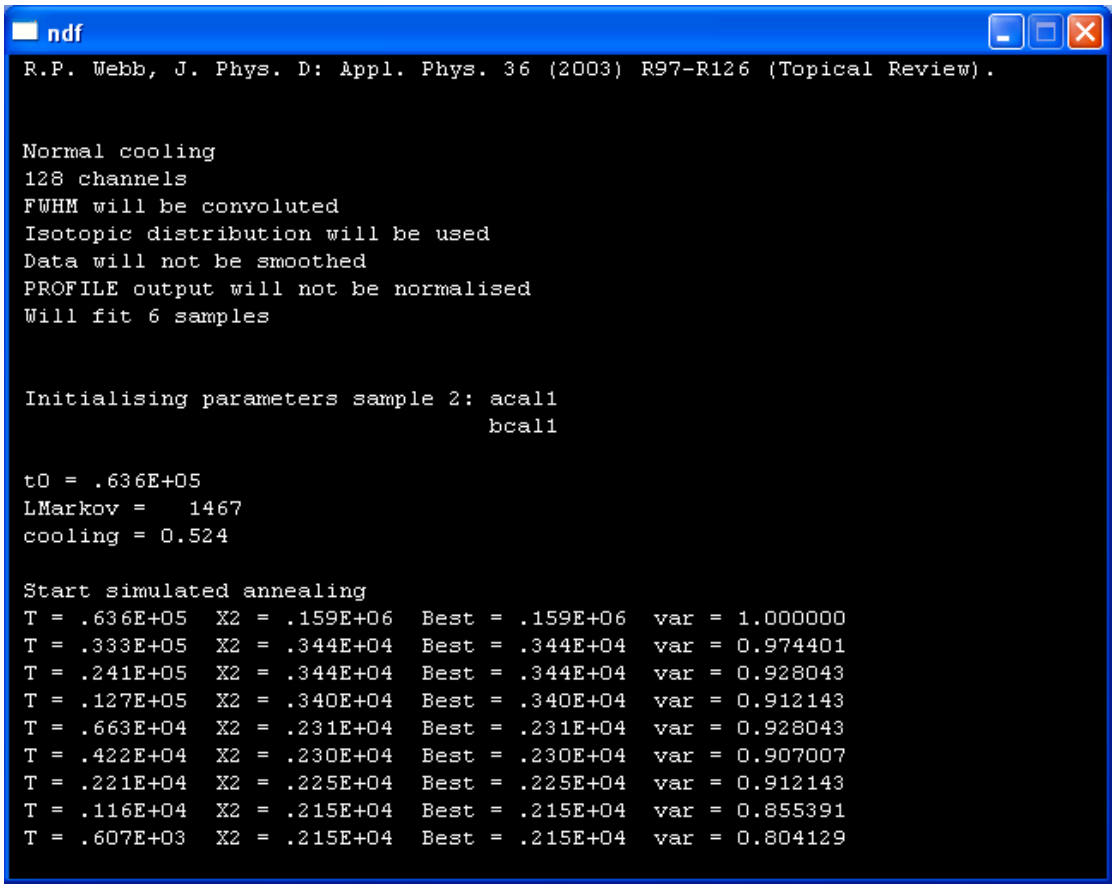
61 Note that substrate does not fit

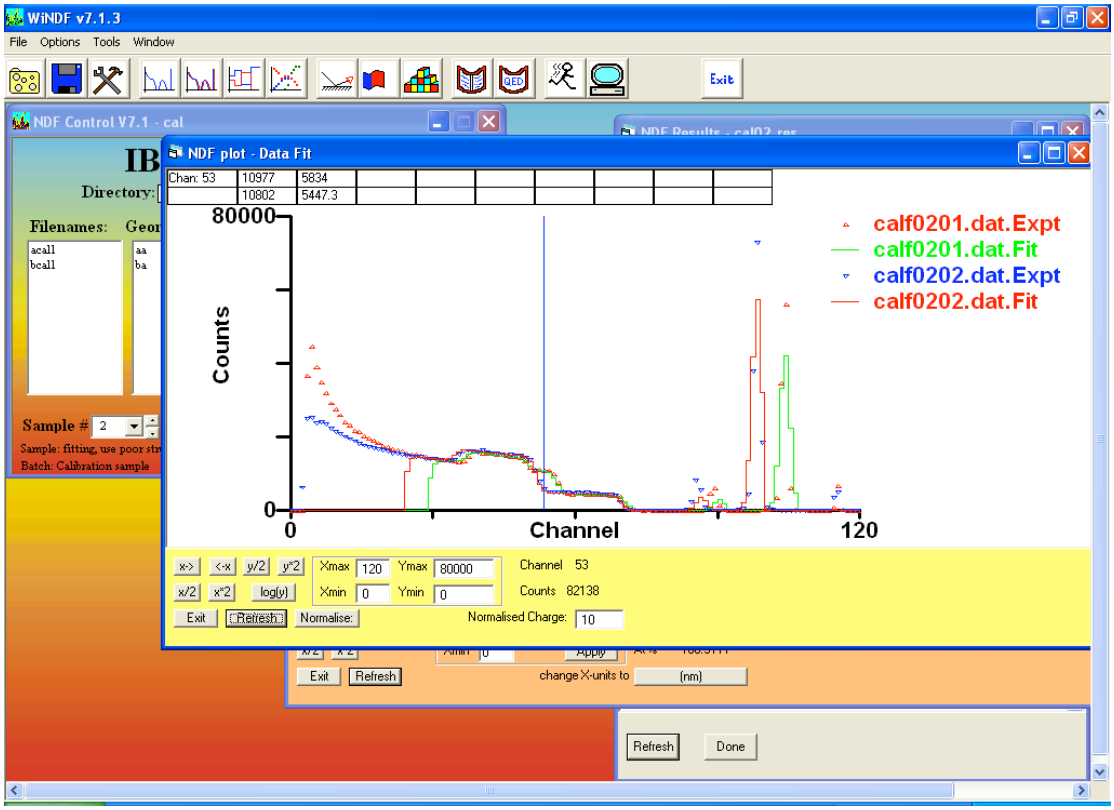
62 Look at fitted structure

63 Inspect output file

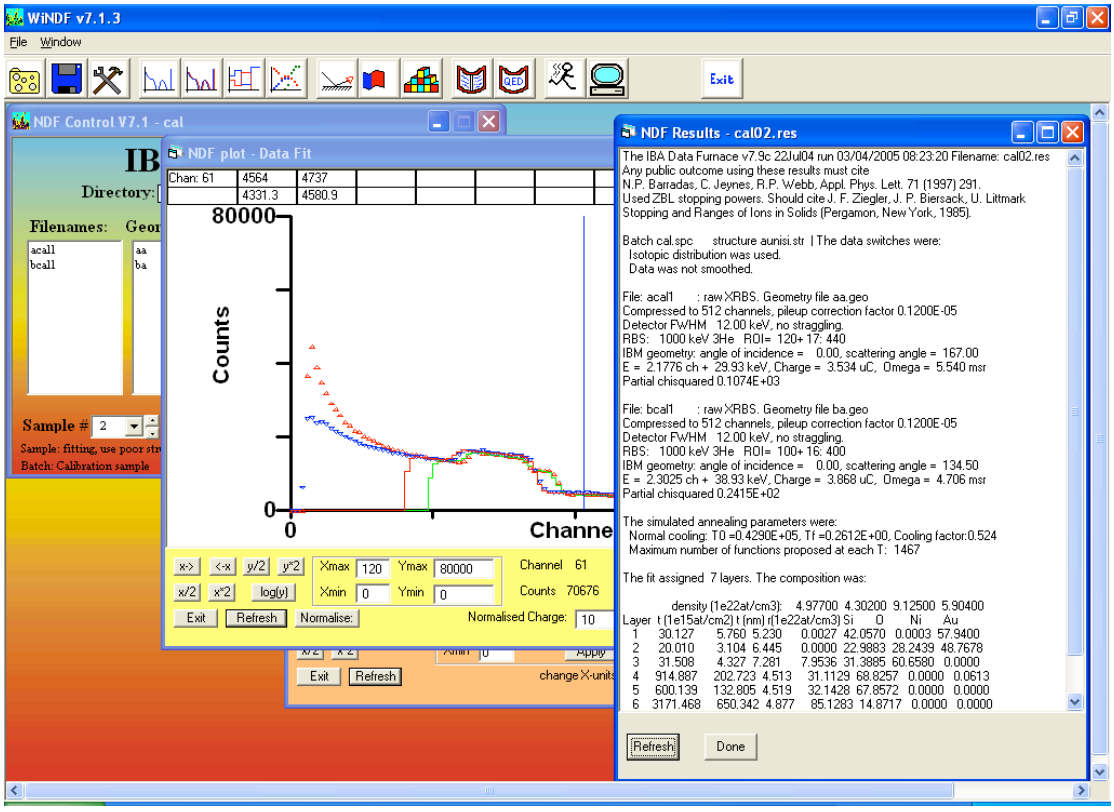


The structure file clearly shows that the O signal runs far too deep! What is wrong? There is a perfectly good fit for the high energy part of the spectrum but somehow a stupid structure is being found! Run NDF, and *while it is running*:



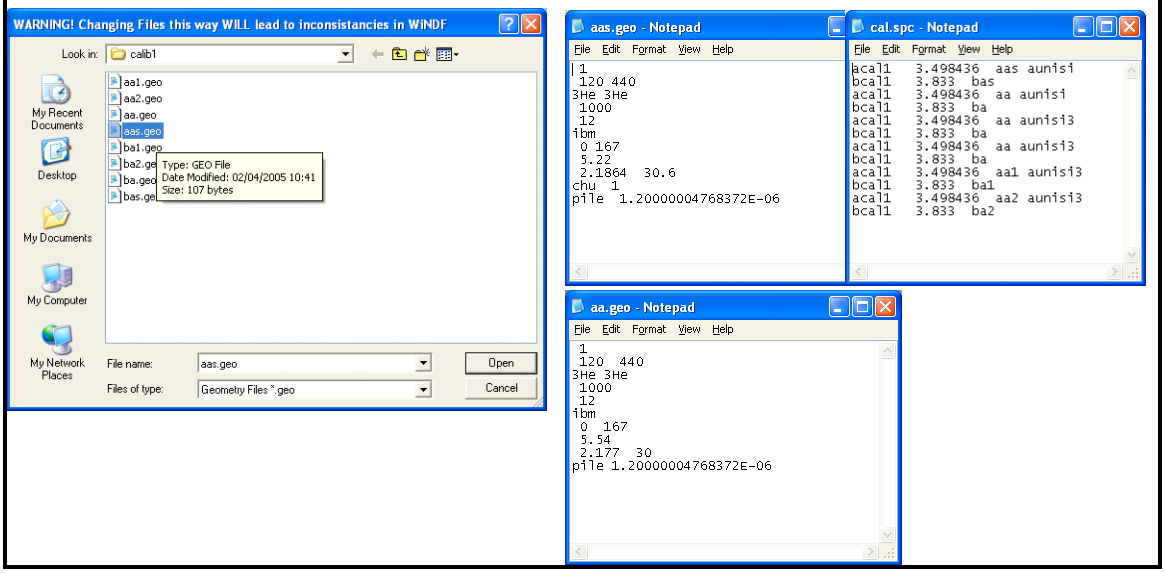


press *refresh* in the yellow screen: this shows the RoIs being used in the geometry files. The data is fitted in the RoI but not outside it (at low energy).

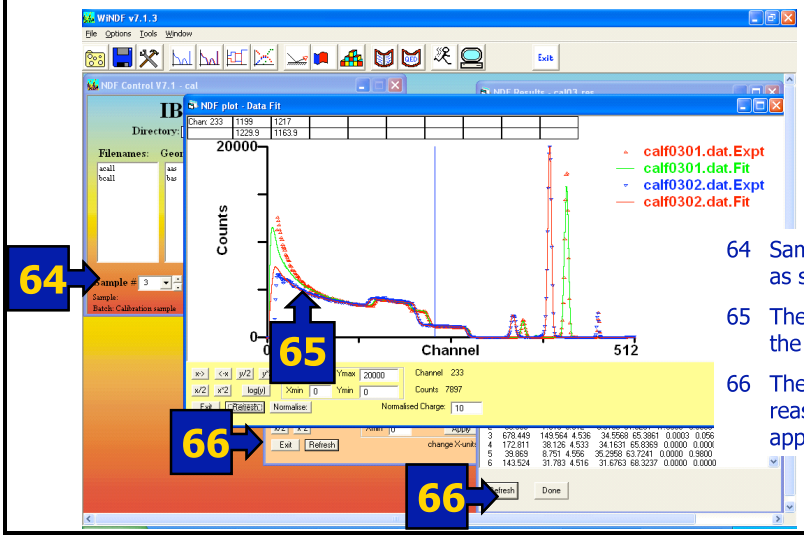


Now inspect the results file. Note that the solid angle ("Omega") is different from Sample 1. Actually we used different geometry files!

Direct inspection of various files



Fitting with NDF: 2



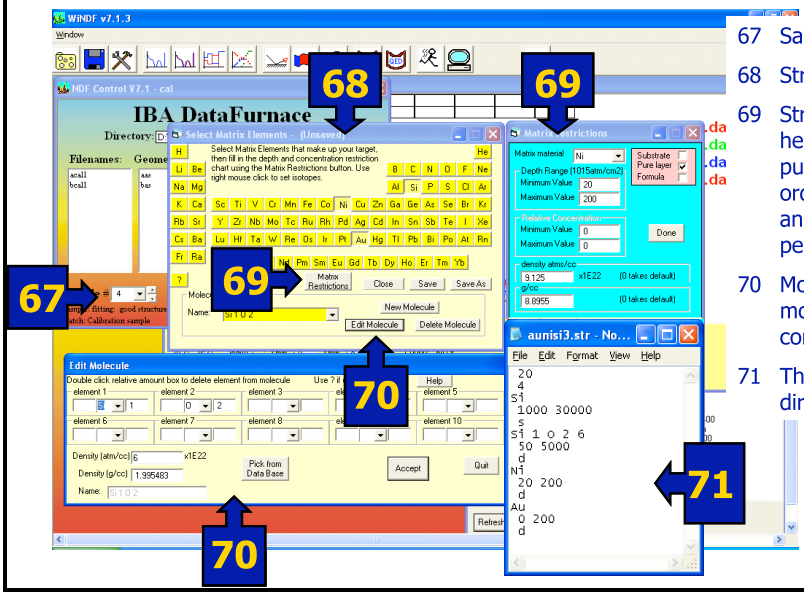
64 Sample 3, with same geometry files as sample 1!

65 The substrate now fits, even outside the RoIs

66 The fitted structure now looks reasonable, and the oxide is approximately SiO2!

The problem now is that the fitted structure does not match what we know about the sample, that it is a layered structure with pure layers and sharp interfaces. The solution found is a *valid* solution *consistent* with the data, but we wish to know if our expected solution (4 pure layers of Au, Ni, SiO2, Si) is *also* consistent with the data. To do this we *restrict the state space* within which solutions are searched for.

Fitting with NDF: 3
Restrictive structure file



67 Sample 4

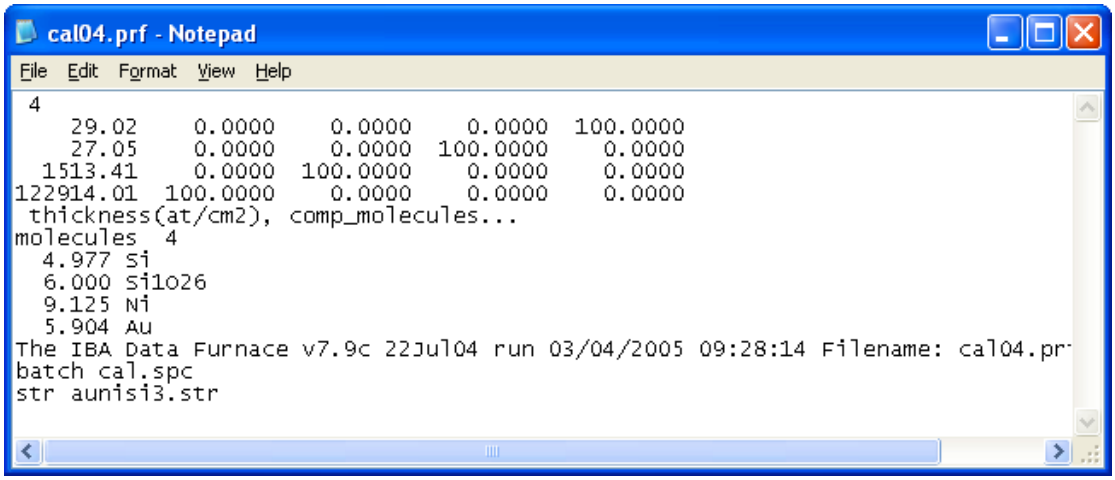
68 Structure file editor

69 Structure file editor second screen: here we can insist that the layers are pure, that they occur in a certain order, what densities are to be used, and what minimum thickness layer is permitted

70 Molecules can be specified with the molecule editor. Note the convenient converter between g/cc and atoms/cc

71 The structure file can also be entered directly using the Notepad editor

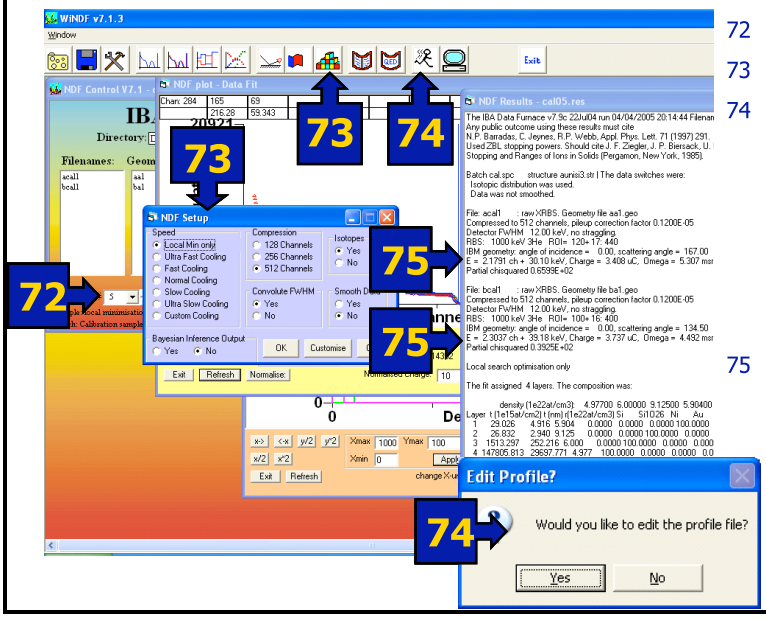
So we can force NDF to find the solution we are expecting. Note that a good fit is obtained, indicating that this is a *valid* solution. IBA data are often *ambiguous*, and in this case the ambiguity is due to the limited energy resolution of the data which limits the film thicknesses that the data can determine. We have effectively told the code that very thin films are present which our systems cannot prove.



You can *look* at the result file using the Notepad editor, and the results are output in a form convenient for putting straight back into the simulator. We can therefore simply store this file as NDF.PRF, and run the simulation.

The point now is that the calibration sample structure is very well known and we want only to verify the calibration parameters. So we don't actually need to do a full fitting, which does not use any knowledge of the sample (except what is in the structure file); a simple local minimisation will do instead. This is much quicker (and needs less attention to the details of the structure file).

Fitting with NDF: 4 Local Minimisation



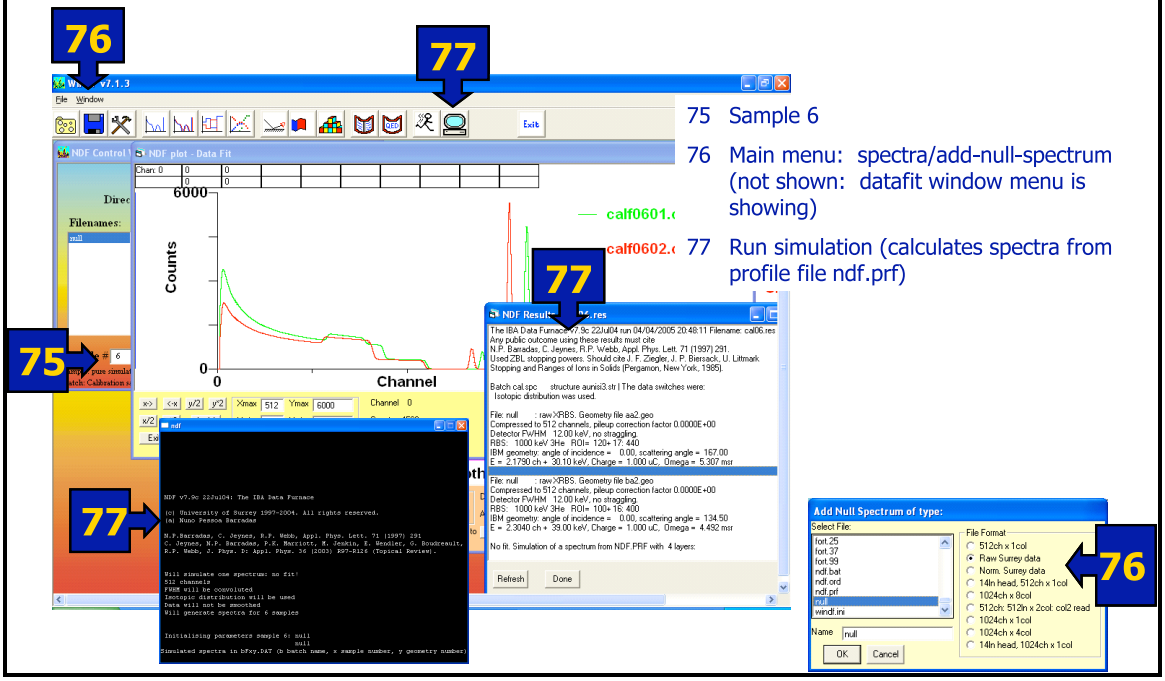
72 Sample 5

73 Select local minimisation

74 Run NDF, which now needs an initial guess. We have already created this file (ndf.prf) by copying the output of the last fit (cal04.prf) to ndf.prf. In any case, we know what the profile file should look like (since the calibration sample is well known) and we could have written it out easily, without doing the fitting step

75 The local minimisation tweaks the calibration values (gain, offset, charge) for the best fit, as well as the layer thicknesses. The values of gain & offset can be copied straight into the geometry files, and the solid angle can be modified to account for the change in the charge

Pure Simulation with NDF



75 Sample 6

76 Main menu: spectra/add-null-spectrum (not shown: datafit window menu is showing)

77 Run simulation (calculates spectra from profile file ndf.prf)

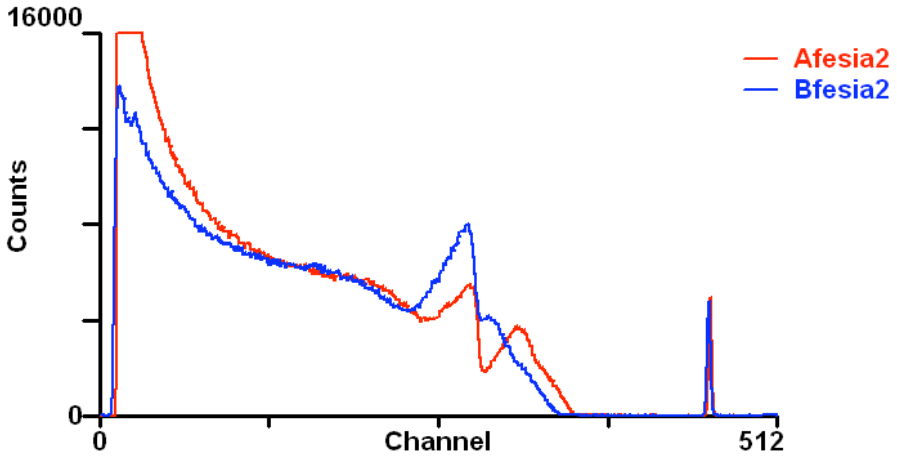
Pure simulation can be used to design analyses and to see what is feasible. Play with it!

Exercise 2: Analysing a batch of data

Open /examples/crest2. This is example 2 on the website www.ee.surrey.ac.uk/ibc/ndf and has been discussed extensively in the *Topical Review*: Jeynes *et al* J.Phys.D 36 (2003) R97

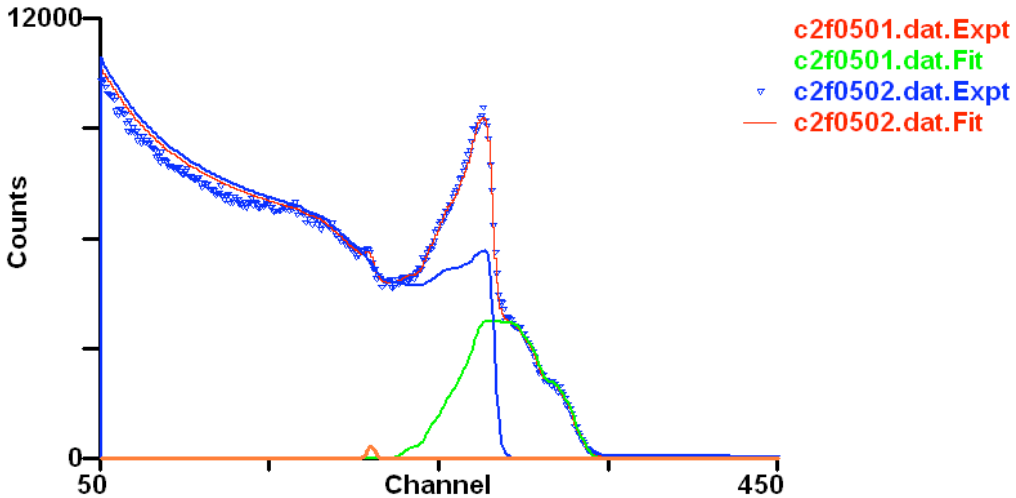
It was the result of a Masterclass involving eighteen year old school leavers, where they analysed an.d wrote up a set of RBS data, which was subsequently published:

A.Belson, D.Brasted, C.Dawes, S.Mashford, H.Sunnucks, J.S.Sharpe, C.N.McKinty, M.Kerford, M.A.Lourenço, A. Kewell, T.Butler, K.P.Homewood, C.Jeynes, R.P.Webb, K.J.Reeson Kirkby, *Ion Beam Synthesised $FeSi_2$ – development of band gap and structure during annealing*, CREST Masterclass project: Presented at ESPRIT Advanced Research Initiative in Microelectronics (MEL-ARI) Athens, October 1999



(This is copied into the document using file/copy on the main menu.)

It shows two spectra collected simultaneously as before, of annealed iron implants in silicon, in a batch of 12 samples with various anneals and implant treatments.



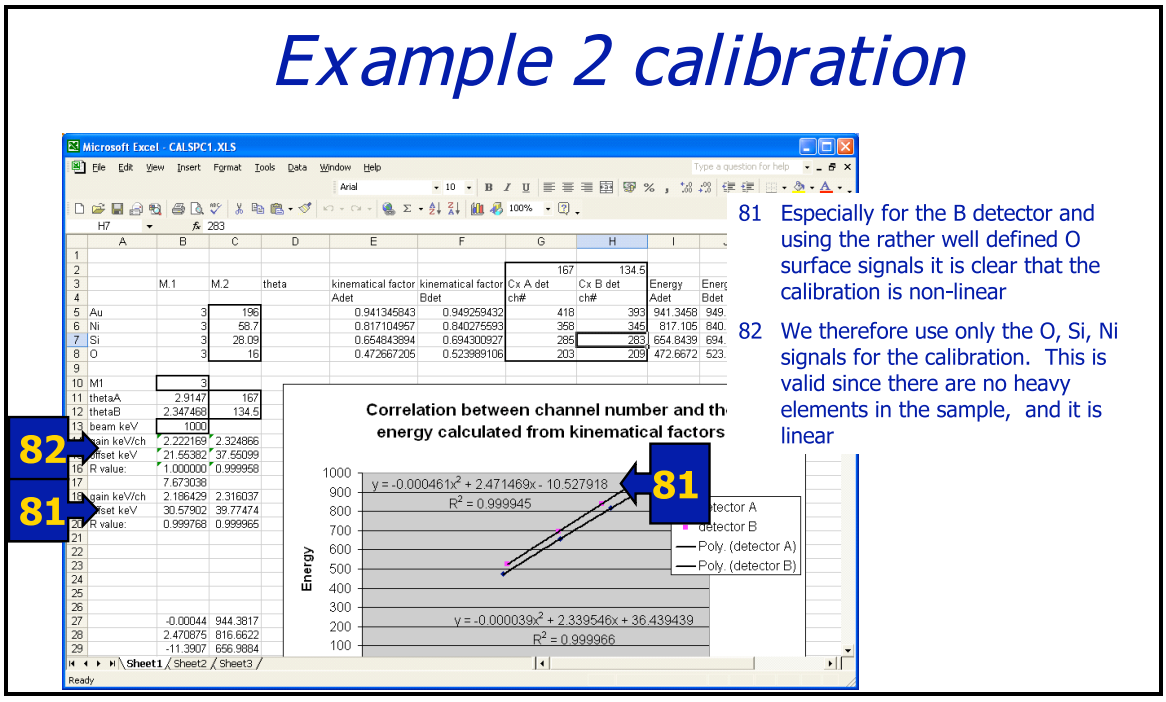
The partial spectra are shown (datafit window menu: file/open-separated-spectra): Fe-green, Si-blue, O-orange. Note the slight channelling below ch.150.

In this case the Fe and Si signals overlap dramatically, making the depth profiles quite hard to extract. We will demonstrate how DataFurnace solves these spectra very easily as a batch.

With an appropriate (not very restrictive) structure file and the correct calibration, the whole batch can be run (runNDF/run_batch).

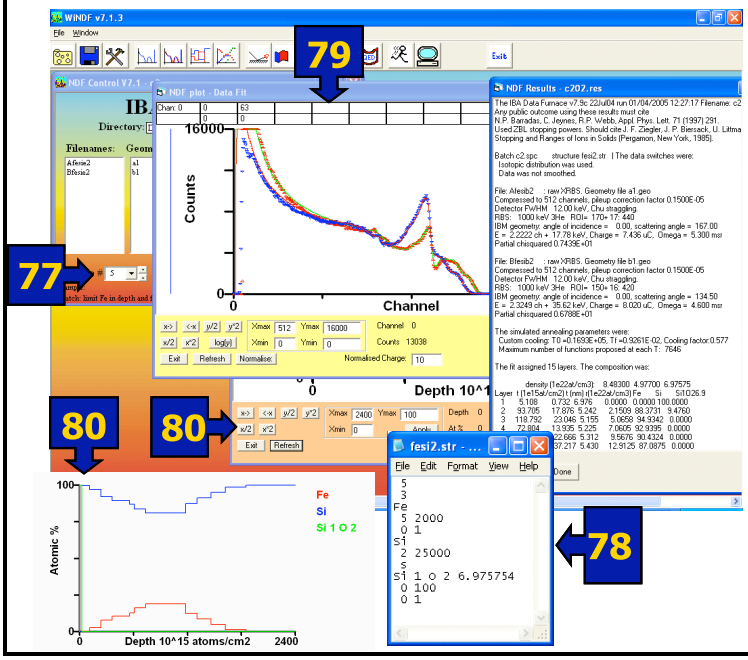
The calibration (gain & offset) is taken initially from the previous exercise (see figure). But they are changed to allow NDF to fit the O signal accurately.

In this case the only well known energy in the spectra is the Si edge (since the Fe is buried and the O signal is very weak). Therefore, NDF does not have sufficient information to adjust the gain & offset, and we hold the gain constant. Because the fits are very sensitive to elemental edge (sharply rising) signals we allow the offset to vary. This will be determined by the Si edge signal.



The solid angles are also taken from the previous spectra, but in general (and in these in particular) the solid-angle.charge product is determined by the spectra, and so we allow the charge to vary. It turns out that the charge collection for this set of spectra is sometimes not very good (compare the collected charges in batch file calib.spc with the fitted charges in c2.spc, most obviously sample 8 in c2.spc).

Fitting with NDF: FeSi samples 1



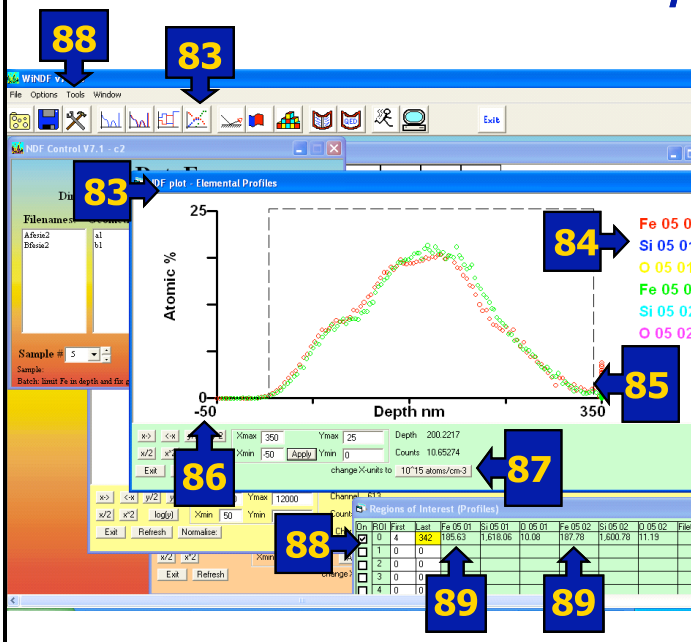
77 Sample 5 has significant surface oxide

78 The structure file allows silica only near the surface, and very thin films

79 This is an excellent fit, done on "ultra-slow", customised to keep gain fixed. Previous runs have adjusted the collected charge to allow good fits

80 The extracted depth profiles fit the oxygen signal with a thin pure oxide, although purity was not demanded in the structure file. Slow fits are needed to fit the O signal convincingly.

NDF: elemental profiles



83 Open the elemental profiles window

84 This has one plot for each element in each spectrum. In this case there are two spectra and three elements, thus six plots. Here, four are invisible (using options/plot)

85 Each plot is obtained by *subtracting* from the *data* all the *calculated* partial spectra *other* than the one in question, and plotting the remainder as depth against concentration. There are therefore 2 *independent* plots for the Fe profile, one for each detector

86 There is signal at negative depth because the finite energy resolution must put some counts from the surface at higher energies (as well as lower)

87 Depth can be plotted in linear units (nm), and this is valid provided the atomic density is correct

88 The numbers of atoms/cm^2 can be counted directly from the data

89 In this case there are 186 and 188.10^{15} Fe/cm^2 for the A & B detectors respectively