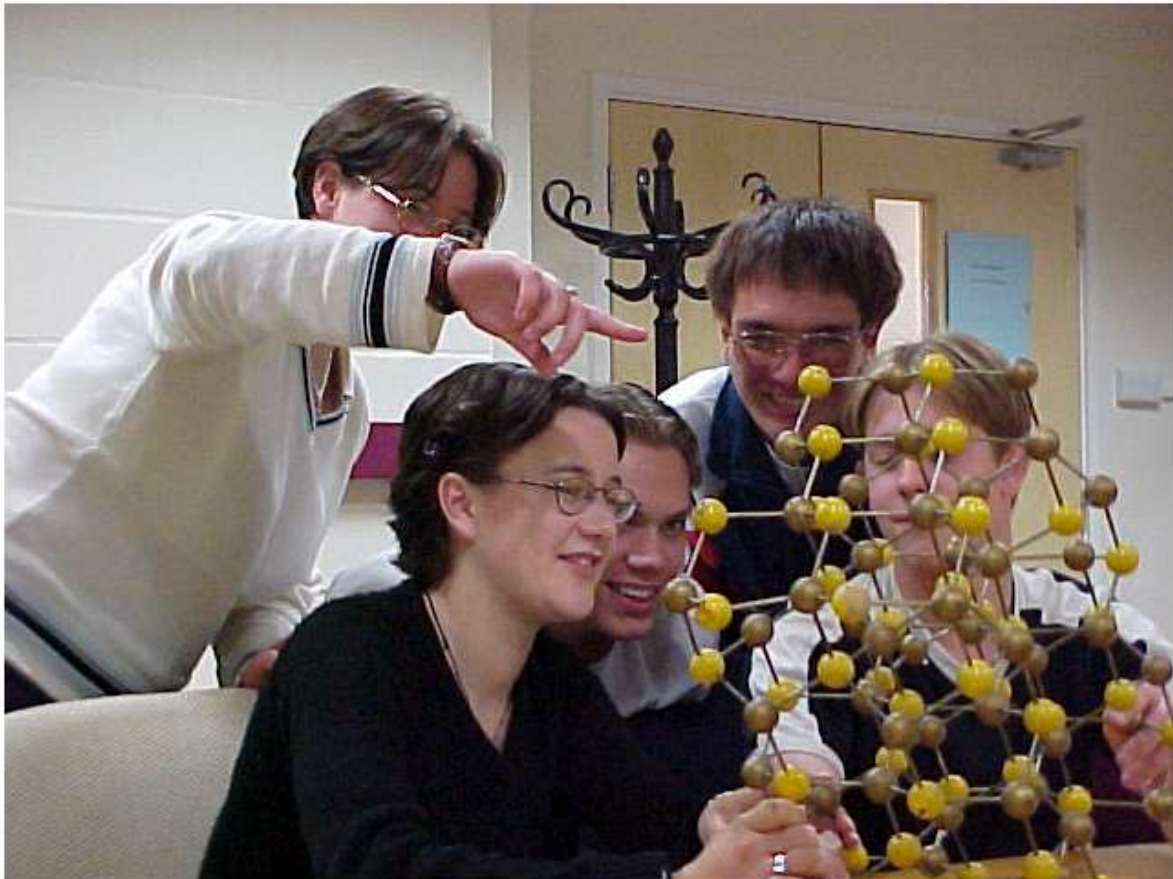


# The IBA DataFurnace v6.5

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**Eighteen-year olds who used DataFurnace to analyse high dose Fe implants in Si (see text)**

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**WINDF: a Windows interface to the DataFurnace code for analysing IBA data**

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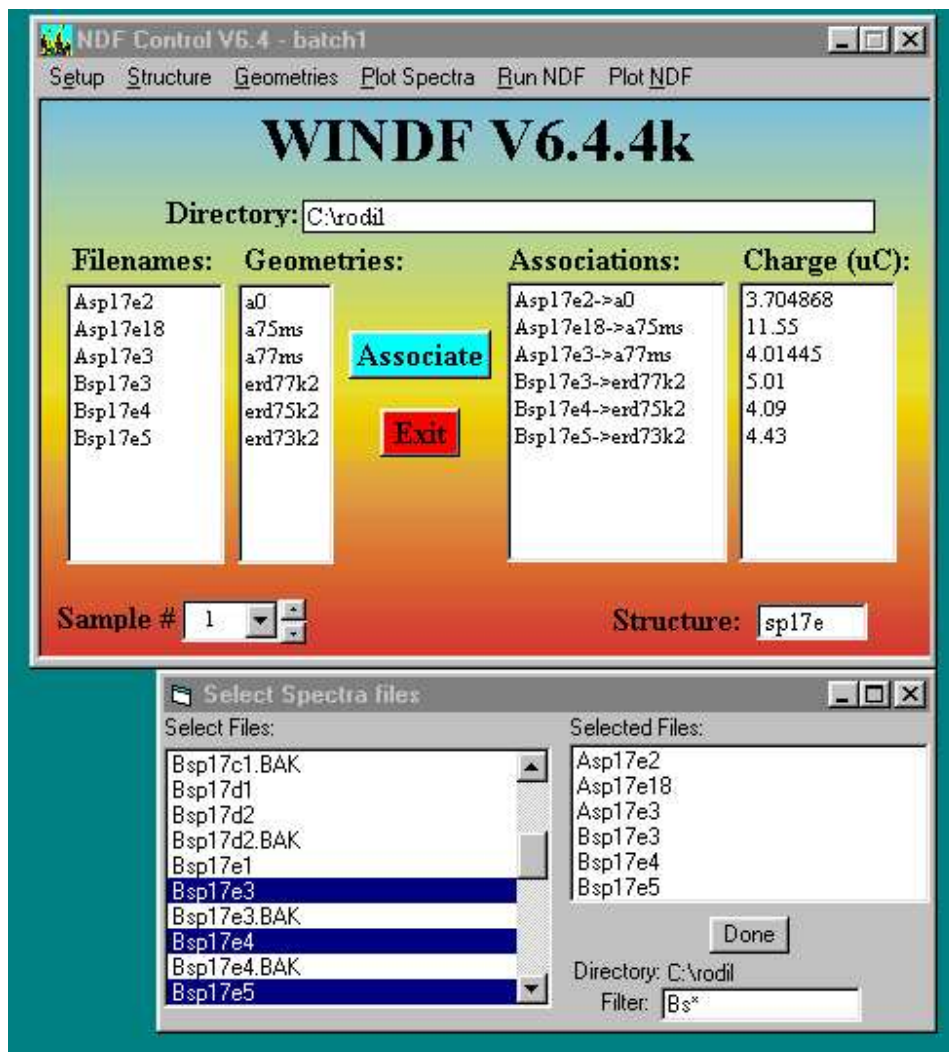
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Recently the inverse problem for Rutherford backscattering spectrometry was solved using the simulated annealing algorithm - the DataFurnace. Since then this code has been generalised to include ERD, a proper calculation of straggle with depth, and self consistent fitting of multiple spectra from the same sample. An ad-hoc treatment of multiple and plural scattering allows data to be fitted closely. A Bayesian code has been implemented to calculate error bars on profiles obtained. Non-resonant NRA data and non-Rutherford scattering are treated correctly and generally.

We have now packaged this code as a Windows program to facilitate the use of NDF on-line and in routine analysis. The input/output has been regularised in a convenient graphical user interface. Spectral analysis tools have been incorporated in an integrated package. The aim is to speed up spectral analysis so that sample analysis can be completed on-line: essential for timely results, or to reveal the need for further data with a different experimental configuration.

The further aim of the package is to encourage the collection of large data sets, with multiple geometry or multiple detector (or both) sample analysis. In the past this was effectively precluded by the time required to extract profiles from many spectra. This package unlocks the power of IBA since it is now feasible to collect many spectra and analyse them immediately and automatically.



**Figure 1: The DataFurnace main window showing a standard file selection sub-window (see text)**

## Introduction

At the last IBA-13 conference we described the recently announced<sup>1</sup> RBS DataFurnace in detail<sup>2,3,4</sup>. This is a code based on the Simulated Annealing (SA) algorithm<sup>5</sup> giving a practical

<sup>1</sup>N.P.Barradas, C.Jeynes, R.P.Webb, Appl.Phys.Lett. **71** (1997) 291-3

<sup>2</sup>N.P.Barradas, P.K.Marriott, C.Jeynes, R.P.Webb, Nucl. Instr. and Methods **B136-138** (1998) 1157-1162

<sup>3</sup>N.P.Barradas, C.Jeynes, M.A.Harry, Nucl. Instr. and Methods **B136-138** (1998) 1163-1167

<sup>4</sup>N.P.Barradas, C.Jeynes, S.M.Jackson, Nucl. Instr. and Methods **B136-138** (1998) 1168-1171

<sup>5</sup>Emile Aarts and Jan Korst, Simulated Annealing and Boltzmann Machines: *A Stochastic Approach to Combinatorial Optimization and Neural Computing* (Wiley, Chichester, 1989)

general solution of the inverse RBS problem (that is, given the spectrum, what is the depth profile?). Since then we have generalised this code to treat ERD (including ToF-ERD)<sup>6</sup>, non-resonant NRA<sup>7</sup> and non-Rutherford backscattering<sup>8</sup>. Therefore we now call it the IBA

DataFurnace although we have not yet implemented PIXE.

A proper treatment of the energy resolution as a function of depth has been given by Szilágyi *et al*<sup>9</sup>, and this is used to permit high depth-resolution data to be extracted accurately<sup>10</sup>. Because the SA algorithm is implemented using Markov Chain Monte Carlo (MCMC) mathematics, Bayesian techniques are natural for calculating confidence intervals on the depth profiles extracted from the data<sup>11, 12, 13</sup>. The intrinsic ambiguity of RBS and related data<sup>14</sup> (not to mention the cost of beam time) implies a pressure to collect multiple spectra simultaneously. We have provided facilities to systematically handle multiple spectra self-consistently at little extra effort to the analyst (examples in most of our latter cited papers).

Because of the intrinsic ambiguity of the data in the general case, extra general facilities have been introduced to exclude unacceptable solutions. A "molecule" option allows the analyst to ask for solutions in terms of the compounds known to be present in the sample<sup>15</sup>: something similar was done previously by Butler<sup>16</sup> but with a completely different methodology. Two other functions have also proved useful in the analysis of complex optical multilayers on float glass<sup>17</sup>: forcing the code to assume pure layers can dramatically reduce the dimensionality of the problem, as can specifying one of the elements (or molecules) explicitly as a substrate.

The DataFurnace code has been made available to the community as a DOS program with no help for the user in the graphics handling of the output<sup>18</sup>. We now describe a Windows package designed to make this output immediately accessible, and including a greatly enhanced

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<sup>6</sup>N.P.Barradas, C.Jeynes, R.P.Webb, U.Kreissig, R.Grötzschel, Nucl. Instr. and Methods **B149** (1999) 233-237

<sup>7</sup>N.P.Barradas, S.Parascandola, B.J.Sealy, R.Grötzschel, U.Kreissig, this conference

<sup>8</sup>C. Jeynes, N.P.Barradas, and J. Wilde, this conference

<sup>9</sup>E. Szilágyi, F. Pászti, and G. Amsel, Nucl. Instrum. and Methods B100 (1995) 103. DEPTH can be downloaded free of charge from <http://www.kfki.hu/~ionhp/>

<sup>10</sup>N.P.Barradas, A.P.Knights, C.Jeynes, O.A.Mironov, T.J.Grasby, E.H.C.Parker, Phys.Rev. **B59(7)** (1999) 5097-5105

<sup>11</sup>P.K.Marriott, M.Jenkin, C.Jeynes, N.P.Barradas, R.P.Webb, B.J.Sealy, CP475, *Applications of Accelerators in Research and Industry* (eds. J.L.Duggan, I.L.Morgan) AIP 1999, pp592-595

<sup>12</sup>N.P.Barradas, C.Jeynes, M.Jenkin, P.K.Marriott, Thin Solid Films **343-344** (1999) 31-34

<sup>13</sup>N.P.Barradas, S.A.Almeida, C.Jeynes, A.P.Knights, S.R.P.Silva, B.J.Sealy, Nucl. Instr. and Methods **B148** (1999) 463-467

<sup>14</sup>P.F.A. Alkemade, F.H.P.M. Habraken and W.F. van der Weg, Nucl. Instr. and Meth. **B45** (1990) 139

<sup>15</sup>M.Milosavljevic, N.Bibic, K.P.Homeood, C.Jeynes, Submitted to Thin Solid Films

<sup>16</sup>J.W.Butler, Nucl. Instr. and Methods **B45** (1990) 160-165

<sup>17</sup>C. Jeynes, N.P.Barradas, R.Close, H.Rafla-Yuan, B.P.Hichwa, Submitted to Surf.Interface Anal.

<sup>18</sup><http://www.ee.surrey.ac.uk/SCRIBA/ndf/>, The DataFurnace Manual, University of Surrey. v1.0 released November 1997, v2.1 released April 1998

core code containing all the facilities mentioned above.

### ***Outline of the DataFurnace code***

The inputs to NDF ("Nuno's DataFurnace") are: the data (the measured spectra), the analytical conditions, any special modifiers to the data, and any restrictions the user wishes to impose on the solution space. We will consider these in turn. Notice that the analyst does not have to make *any* initial guess at the solution, nor does he have to input any sort of layer structure. This is a fitting, not a simulation code, although access to standard simulation is naturally built in. The stopping power database used is given in a standard format in separate files.

The outputs are: a text file of the results giving a summary of input files and conditions used and the layer structure of the solution found, a text file logging the progress of the calculations (including start and end times). Text files (also suitable for input to other graphics programs) are also output showing: data and fits, that is the measured spectra and the spectra calculated from the best fit solution (including how the fits are made up from different elemental signals). The solution obtained is also output as an elemental concentration in at% against depth in atoms/cm<sup>2</sup>, as is a utility for showing the measured histogram data directly on a depth scale.

NDF takes the input data and searches systematically through solution space for a solution consistent with the data. IBA data may be badly ambiguous, and the analyst may have to exclude parts of the solution space to avoid the choice of valid but unacceptable solutions by the code. We have developed a series of general tools to facilitate this.

The use of NDF generates a very large number of files (for example, the analysis of 22 CN<sub>x</sub>:H samples has left a directory with well over 2000 files), and to provide a convenient GUI (graphical user interface) for the analyst we have developed WiNDF ("Windows NDF").

### ***WiNDF: Overview***

Fig.1 shows the main window of WiNDF. NDF works in a single directory shown in the Directory box. There are six spectra to be analysed simultaneously, all taken from this sample #1 with the experimental conditions given by the Geometry files and the sample elements given by the Structure file. The user selects the spectra and the geometry files required with a standard dialogue box, and then associates a geometry with each spectrum. In this case glancing incidence RBS spectra (at 2 angles) and ERD spectra (at 3 angles) together with a normal incidence RBS spectrum were all collected for the same sample. The collected charge is read from the data or entered by the user, and all this is saved in the Batch file "batch1" (in the banner). Similar information for further samples can be added to the batch file. Fits for individual samples or for the whole batch (or sub-sets thereof) can be run. Simulations for

specified layer structures are also convenient to run and display.

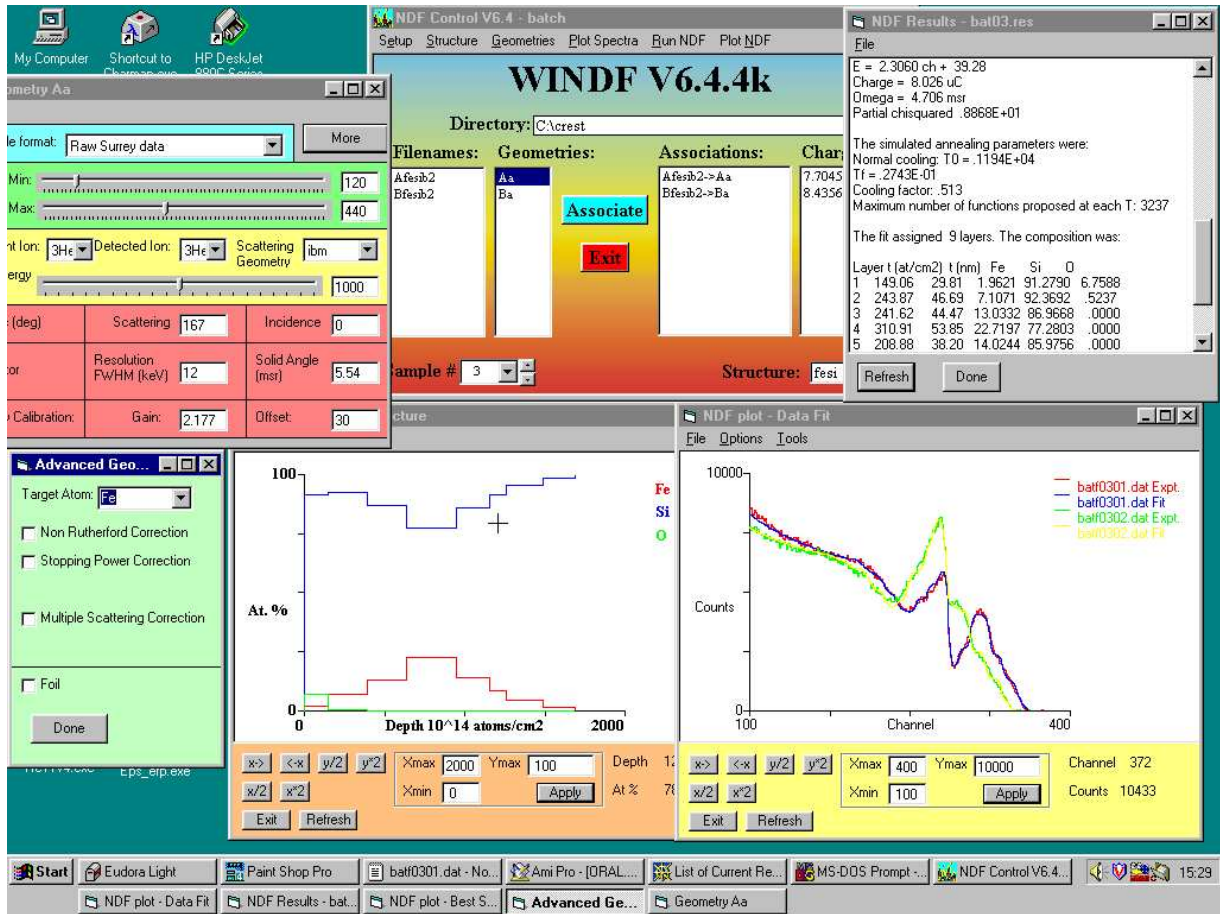
### ***Use of WiNDF to solve complex IBA data***

Fig.2 is an example of how WiNDF can be used by the inexperienced to extract information from complex RBS data. These data came from an investigation into the ion beam synthesis and annealing behaviour of  $\beta$ -FeSi<sub>2</sub> carried out by a group of eighteen year olds under the "CREST" Masterclass scheme<sup>19</sup>. Qualified staff collected the data and set up the geometry files, but the students carried out the data analysis and obtained depth profiles for a large set of 12 samples, essentially unaided, in less than a day.

Numbering the windows in Fig.2 clockwise from top left, the main window is #2, and sub-window #4 is the starting data (two spectra collected simultaneously from 2 detectors at 167 and 135 degrees scattering angle) together with the fits obtained which are so close as to be almost indistinguishable from the data. Sub-window #5 is the solution obtained: a depth profile in at% versus depth (in thin film units) for each element of the sample; this is a graphical representation of the NDF output shown in sub-window #3. Sub-window #1 shows the contents of one geometry file: this data is for a 1MeV <sup>3</sup>He<sup>+</sup> beam, and NDF needs the beam geometry, detector energy resolution and solid angle, and the electronics gain calibration to interpret the data. The geometry file also contains information to apply various corrections, and information about the range foil (for forward recoil work) (sub-window #6). Note that with this beam much of the Fe signal overlaps the Si signal: we could have used a different beam to separate the signals but this beam was convenient in this case for operational reasons.

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<sup>19</sup><http://www.ee.surrey.ac.uk/crest/brigade.htm>; 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, to be presented at *ESPRIT ADVANCED RESEARCH INITIATIVE IN MICROELECTRONICS* (MEL-ARI) Athens, October 1999

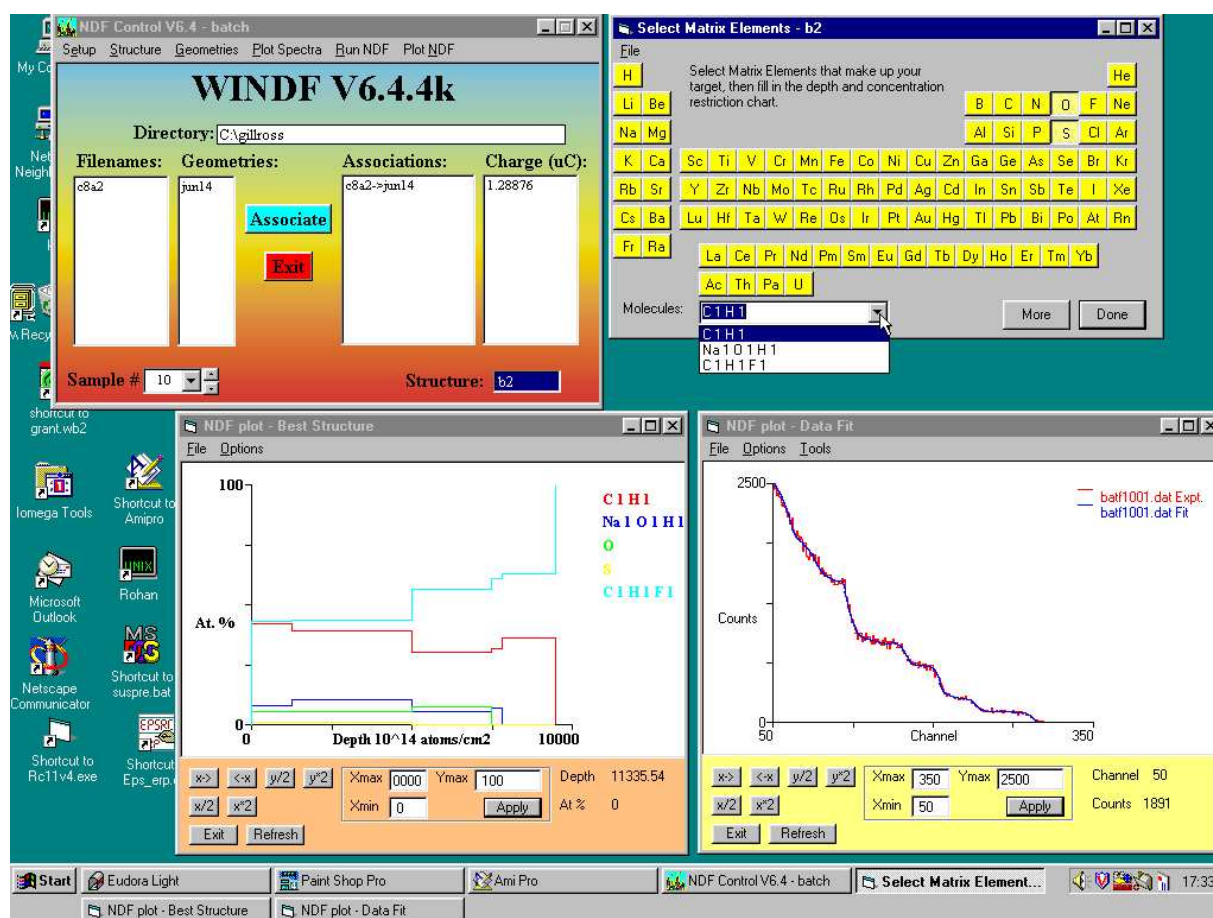


**Figure 2: 1 MeV  $^3\text{He}^+$  RBS of Fe implants into Si, with annealing, as analysed by school-leavers.** Numbering the windows clockwise from top centre: 1) Main window showing filenames of the spectra to be analysed, filenames of the geometry files, the associations of the spectra with the geometry, and the collected charge for each spectrum. The elements of the sample and any solution space restrictions are in the structure file. Multiple samples can be analysed, with all this information stored in the Batch file. The sub windows are: 2) NDF results are output as a text file. 3) The data and the spectra calculated from the fitted solutions are almost indistinguishable. 4) The depth profile plotted graphically. 5) a sub-window of: 6) The "geometry" sub-window with beam details, sample and detector geometry, detector resolution and electronic gain etc.

Note that this mode of data presentation is its own validation since the quality of the fit is presented together with the solution. Note also that the use of a double detector analysis greatly adds to the confidence in the result since the fit is consistent with both spectra.

Figure 3 is a different type of case. This is single detector data collected from a polymer film mounted on a cold stage to minimise beam damage. However, we are looking for near-surface changes to the film due to its treatment. The bulk film is of composition (CHF), and the treatment is expected to effectively turn the surface into (CH) with some other molecules around represented by free O, S and sodium hydroxide (from the treatment solution). This sort of data is notoriously ambiguous because the light elements can exchange for each other giving a wide

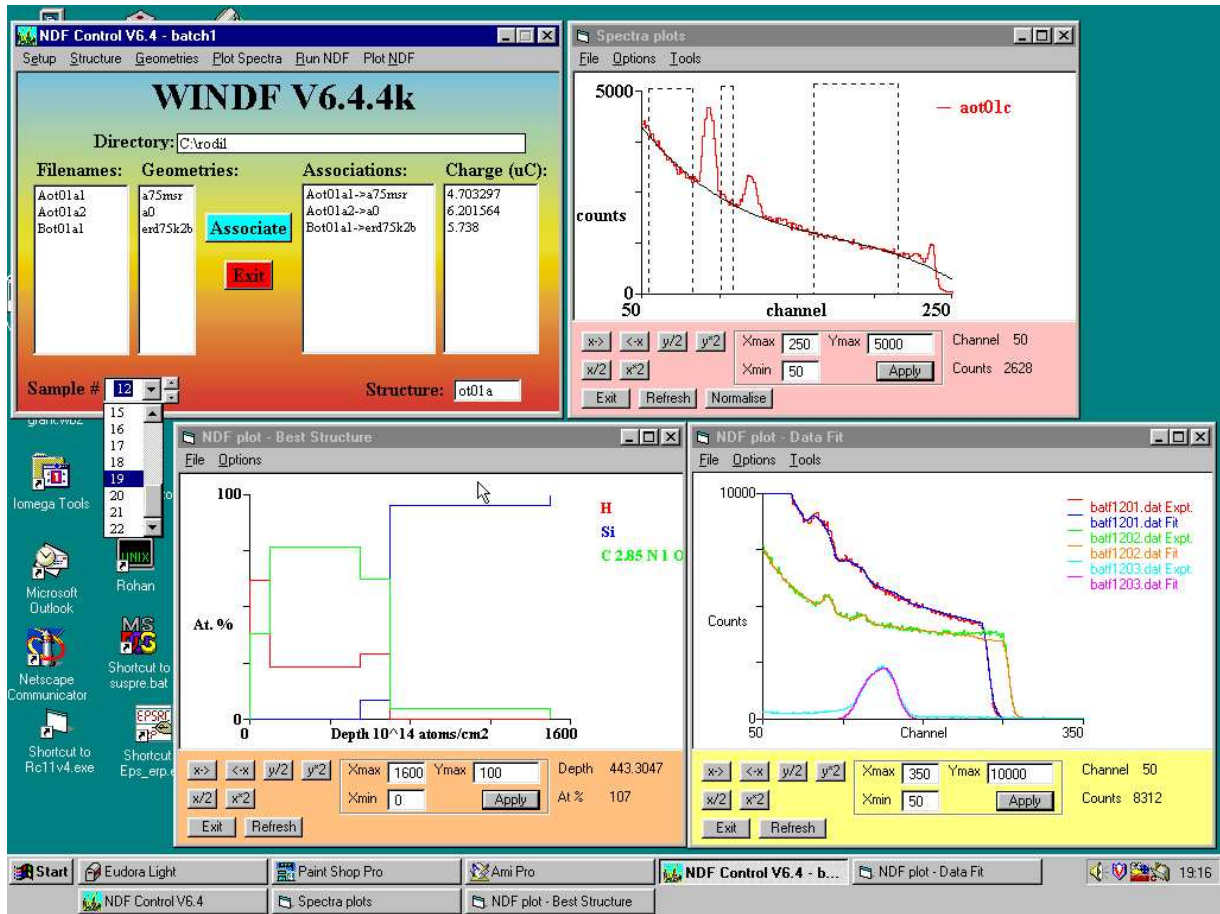
range of valid "solutions", and we need to find a way of correlating the signals from different parts of the spectrum. We can give DataFurnace molecules instead of elements to construct trial solutions with: in this case the structure specifies three molecules and two elements (5 free parameters and 6 different elements in the sample, one of them - H - invisible to RBS). The solution clearly shows the substrate molecule (CHF) losing fluorine towards the surface. DataFurnace is very convenient for this sort of problem, since different parametrisations can easily be tried to see if realistic constraints on the solution space can actually yield an unambiguous solution.



**Figure 3: RBS/ERD data of  $CN_x:H$  films using C:N ratios from RBS-c measurements.**

1.5MeV normal incidence  $^4\text{He}^+$  RBS of a fluorinated polymer after immersion in a defluorinating solution for eight hours. The structure file specifies the elements and molecules to be used in the fit.

Figure 4 shows our final example: this is of a set of  $CN_x:H$  films deposited on silicon where the composition was required. This can be obtained quite easily with a 1.5MeV He beam by using ERD with a semiconductor detector and a suitable range foil simultaneously with RBS. The data and fit are shown in the bottom right sub-window. There is a problem with this type of data however: the C and N signals have a rather small signal to noise ratio due to the substrate signal background. Therefore we determined the C:N ratio separately by a normal incidence analysis where the beam was aligned with the substrate thereby dramatically enhancing the signal to noise ratio (data is shown in top right sub-window, with a cubic fit to the regions of interest shown: there is also some O in this film). Then this value was supplied as a molecule to the RBS/ERD data, with the result in the bottom left sub-window (C/N=2.85). The data is distorted by the large low energy tail on the H ERD signal due to multiple scattering (this can be minimised by suitably truncating the data given to NDF - see the "min" & "max" boxes in the geometry window of Fig.2), and also by small channelling effects in the RBS signal. However, even with these reservations a reasonable self-consistent fit is obtained. Again, as the drop down selection box in the main window shows, this batch is of 22 samples; and since the fits are done without manual interference the analysis is completed quite objectively.



**Figure 4:** 1.5MeV  $^4\text{He}^+$  RBS/ERD data of  $\text{CN}_x\text{:H}$  films using C:N ratios from RBS-c measurements. C/N = 2.85 is determined from a channelling measurement (top right window). simultaneous RBS/ERD spectra (glancing beam incidence) and an RBS spectrum (normal incidence).