Application Note: 31005

The *Avantage* Data System

Key Words

- Surface Analysis
- Batch Processing
- Data Acquisition
- Data Processing

Introduction

The purpose of this document is to provide an overview of the Thermo Scientific *Avantage* data system. Many of the key features are described but, in order to keep the document to a reasonable length, many of the features of *Avantage* have been omitted.

The Operating System

The *Avantage* data system for Thermo Scientific surface analysis equipment is based upon the Windows® operating system. Being based on this industry-standard operating system provides many advantages including:

- Most users are familiar with Windows software and operation of *Avantage* is therefore more intuitive.
- Tools provided in the operating system allow for rapid and convenient use of third-party software packages. For example, copy and paste functions facilitate report generation.
- The operating system allows the user to customize their desktop to suit their requirements. For example, toolbars can be configured with the user's choice of icons.
- Security is improved by allowing different levels of user access to different parts of the software. Expert users can have access to parts of the software which allow the instrument parameters to be set. Occasional or novice users are restricted to data collection, using a selection of pre-set parameters, and data processing. The system is easily protected with passwords.
- Many users work with a Windows-based network. It is therefore a simple task to connect the *Avantage* data system to the users' network.

Acquisition

Avantage controls all aspects of data acquisition, where appropriate, these include:

- Sample alignment
- The spectrometer and its associated lenses and detector
- Monochromatic and non-monochromatic X-ray sources
- Field emission electron gun
- Ion gun
- Flood gun

Sample Alignment

XPS

The image from the system microscope can be displayed on the desktop. From this image, the positions for analysis can be selected. Figure 1 shows the view from the optical microscope displayed in an *Avantage* window. In this case, a marker is displayed showing where a line scan is to be performed. The optical image can be stored for inclusion in a report.

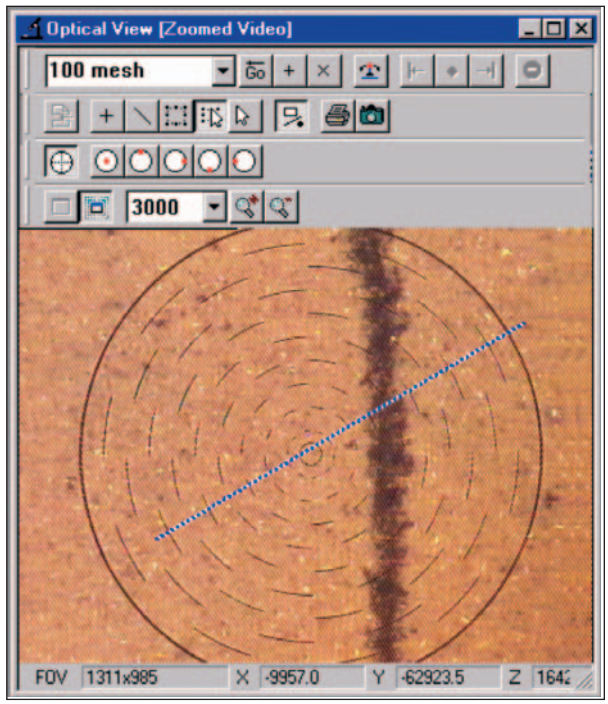

Figure 1: Optical view of the specimen from which the analysis position can be selected. The line on the image shows the location of a line scan which is about to be acquired

The point of interest can be moved to the analysis position at the centre of the image. Alternatively, a point on the optical image can be selected with the mouse and that point will then be moved to the analysis position. If multi-point analysis is needed, several positions on the optical image can be selected and they will be analyzed in turn.

Auger

When using scanning Auger, the analysis positions and types can be defined using the SEM image or (if the optional detector is fitted) a backscattered electron image.

Figure 2 shows an example of an SEM image, acquired from Thermo Scientific MICROLAB 350, with analysis positions marked on it. The image shows two positions at which a point analysis has been defined, a position at which a line scan is to be acquired and the position and size of an Auger image acquisition.

Figure 2: SEM image of part of a steel sample with analysis positions superimposed on the image

The Experiment Tree

All of the experimental parameters can be controlled, in any combination, in a single experiment using the concept of the experiment "tree", illustrated in Figure 3.

The various parts of an experiment are defined as "objects" on the tree. As the experiment continues, the instructions contained within each object are performed. If there is a branch at any given object the instructions contained within the branch are performed before moving on to the next object at the same level in the hierarchy.

The structure of the tree is similar to that of the directory in Windows Explorer. Sections of the Experiment Tree can be copied and pasted or imported from other experiments, in the same way that files or folders are moved within Windows Explorer.

In the example shown in Figure 3, the first action is to set the X-ray source to 15 kV, at a power of 150 watts and a spot size of 500 µm.

The next object moves the manipulator so that the sample 1 is in the analysis position. A survey spectrum is then acquired.

Once the survey scan from sample 1 is complete, sample 2 is moved to the analysis position and further spectra are acquired, a survey spectrum followed by narrow scans from Si 2p, C 1s, N 1s, O 1s.

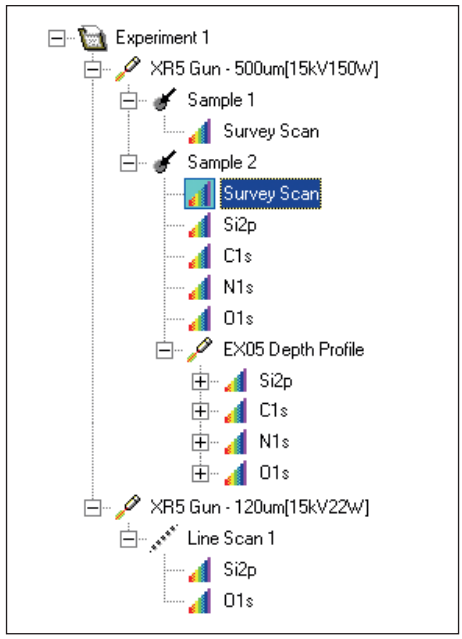

Figure 3: Example of an experiment tree

A depth profile is then performed at the same position.

On completion of the profile, the spot size of the X-ray beam is reduced to 120 µm and an XPS line-scan is acquired.

Other objects, not shown in this example, would control the electron gun, image acquisition etc.

Object Properties

Once the structure of the tree has been set, the properties of each object are defined. This is achieved by selecting the appropriate object (the highlighted survey scan in the example in Figure 3) and displaying a property dialog box with a right click on the mouse.

In this case, a scanned spectrum has been selected with the analyzer set to a pass energy of 100 eV. The energy range for the scan, step size and dwell time for each step are also set in this dialog box. This box is also used to select between CAE and CRR modes of operation as well as selecting the required lens mode.

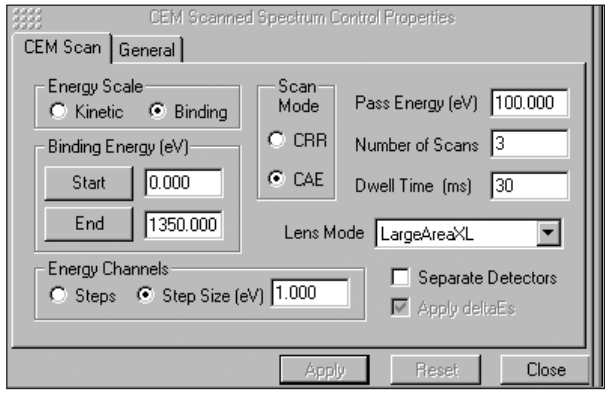

Figure 4: A spectrum property dialog box, in this case set for survey spectrum

Analogous dialog boxes are displayed for each of the types of object on the experiment tree. For example, the one associated with the X-ray source has the following controls:

- Source selection (monochromator or twin anode)
- If the twin anode source is to be used then the anode material is selected
- Anode power
- Spot size for a microfocusing monochromator

The whole experiment tree and the properties of each object can be stored for use on later samples and all of the acquisition parameters are stored with the data.

Batch Processing

The experiment tree can be used to define data processing as well as acquisition. An example is shown in Figure 5. In this example, an X-ray spot size of 400 µm is selected and sample 1 is moved to the analysis position. Following the acquisition of spectra, a peak table is opened so that the data can be quantified. The peaks are then fitted after which the peak table and fitted spectra are exported to a Microsoft Excel spreadsheet. The spreadsheet can be configured such that it includes a page which summarizes of all of the data collected in the experiment. This could consist of a table showing the atomic concentrations of the elements included in the acquisition.

Sample 2 is then moved to the analysis position and the process is repeated.

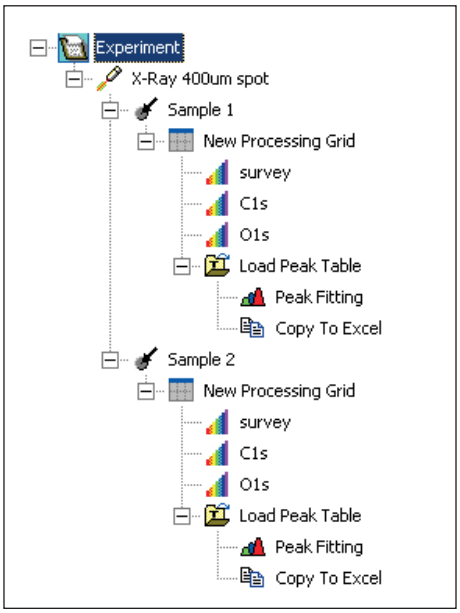

Figure 5: An example of an experiment tree containing data processing

This example shows only a limited number of processing steps, others such as non-linear least squares fitting and printing are also available as processing steps.

Once the experiment is set up, this powerful feature allows truly unattended operation of the instrument.

Processing

Avantage has a comprehensive set of data processing tools. All processing steps are recorded as an audit trail leading from the originally acquired data. It is not appropriate here to describe all of the facilities available in *Avantage* but some of the more important ones will be described.

Peak Identification

The data system has an integrated library of peak positions and relative intensities. This library can be used either automatically or interactively to identify peaks and to quantify the spectra. Figure 6 shows a screen which is displayed when using the interactive peak identification.

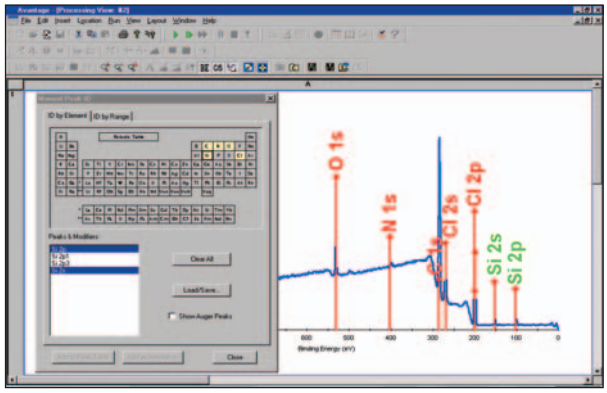

Figure 6: The use of the periodic table to obtain stick spectra as an aid to peak identification

Quantification

Identified peaks are automatically added to a peak table which can then be used for quantification.

For quantification purposes, the data system has integral libraries of relative sensitivity factors (both Scofield and Wagner) the user simply selects the required library. Alternatively, customized libraries can be created using data from standard samples.

All data files contain information about the acquisition conditions, including the spectrometer conditions. From this information, the quantification routine automatically applies the correct instrument transmission function to the data.

Peak Fitting

A fast, versatile and interactive peak fitting facility is part of the *Avantage* processing software.

This part of the software controls the number of peaks, peak position, peak width, Gaussian/Lorentzian (G/L) ratio. The type of background is selected by the user (linear, Shirley or Tougard). Linking and fixing of peak parameters is simple and asymmetric peaks can be fitted when required.

The original data is displayed along with the individual fitted peaks, the overall fitted spectrum and, optionally, the residual spectrum.

The routine also generates a peak table which is used for quantification.

Figure 7 is an illustration of an *Avantage* screen during peak fitting. In multi-level data sets (eg profiles, linescans ARXPS), it is possible to fit every level rapidly and conveniently using the same parameters and constraints.

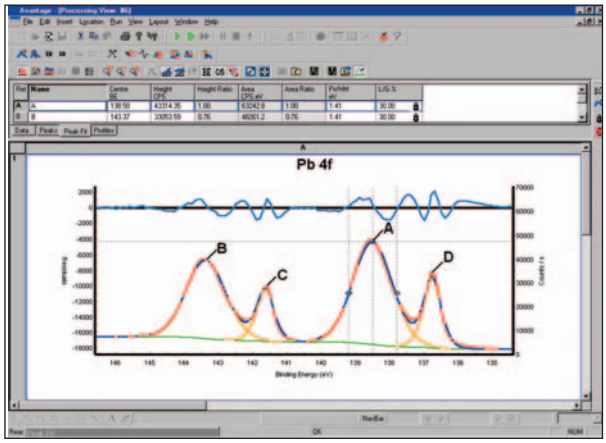

Figure 7: The screen displayed during peak fitting

Non-Linear Least Squares Fitting (NLLSF)

When the data contain sets of spectra (depth profiles, linescans, angle resolved XPS etc.) it is often appropriate to use the combination of Target Factor Analysis (TFA) and Least Squares Fitting. By these means, subtle differences in the spectra can be used to determine the way in which various chemical states change within the data set.

In some experiments there is an energy shift in the data. Under these circumstances NLLSF can be used so that a charge shifted peak is not treated as a different chemical state. A typical screen, displayed during the NLLSF routine is shown in Figure 8.

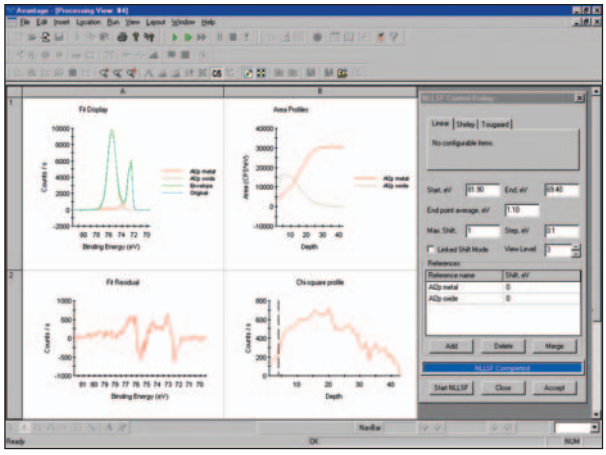

Figure 8: A typical screen which is displayed when NLLSF is being applied to a data set

Angle Resolved XPS

Avantage is able to process ARXPS data in a number of ways. For an explanation of the principles on which this part of the software is based, refer to application note 31014.

Relative Depth Plot

This is the simplest treatment for ARXPS data and shows the ordering of layers within an ultra-thin film. The plot is constructed for each species by taking the logarithm of the ratio of the XPS peak area at near grazing emission angle to that at near normal emission. Figure 9 shows an example of a relative depth plot from hafnium oxide on silicon oxide on silicon. Carbon, a surface contaminant, can be seen nearest to the surface while the elemental silicon is deepest in the structure, as expected. In addition, it can be seen that oxygen exists in two chemical states, each having a different depth distribution, one is associated with the hafnium (O 1s Low BE) and the other with the silicon.

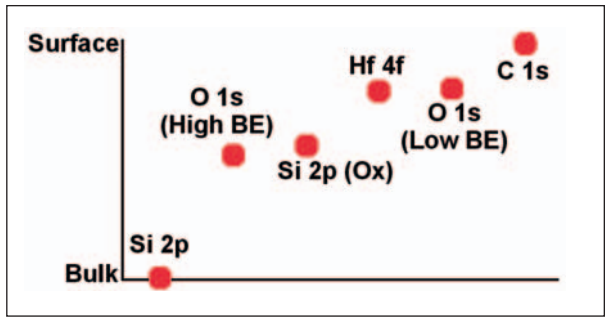

Figure 9: Relative depth plot from a hafnium oxide film on silicon dioxide on silicon

The relative depth plot has the advantage of being independent of any model and does not require the knowledge of the physical constants for the material. It can show, for example, the change in position of a species due to some form of treatment, such as annealing.

Multiple Overlayer Calculator

This part of the software calculates the thickness of up to 3 layers on a substrate using the angle resolved XPS data. Figure 10 shows the calculator. The user selects the number of layers whose thickness is to be calculated (1, 2 or 3), an XPS peak representative of each one and the identity of each of the layers. From a database of the relevant physical properties (e.g. density and band gap) the software calculates the attenuation length for each of the electrons. When the "Calculate" button is pressed a least squares fitting routine is applied to the data to calculate the thickness of each layer. A graph displays the experimental and calculated data so that the user can inspect the quality of the fit.

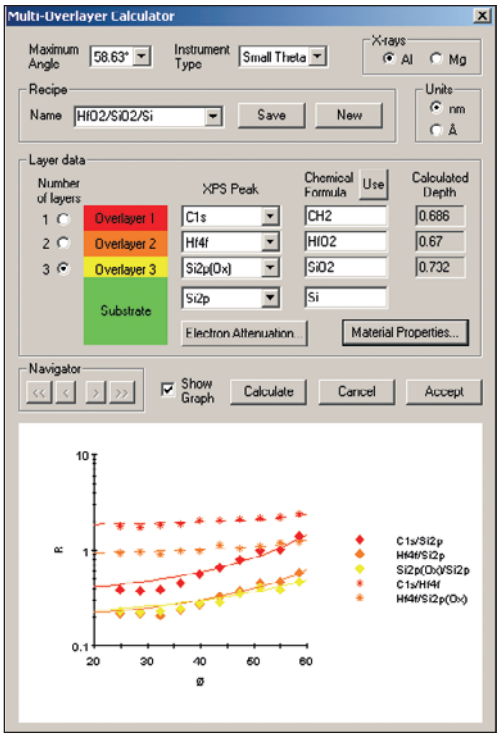

Figure 10: Screen shot of the multiple overlayer calculator

If the database values for the physical properties or the calculated ARXPS parameters are not appropriate, the user can insert the values thought to be most appropriate. It is possible to save all of the input parameters as a recipe which can be applied to other data sets.

Depth Profile

Using iterative methods involving Maximum Entropy and/or Genetic Algorithms it is possible to construct a depth profile from ARXPS data. Figure 11 shows the window used for the construction of a profile. In this case, the process is using the Genetic Algorithm to construct the profile. All methods are iterative and, when Figure 11 was acquired, the iterative process had further to run to achieve the optimum fit to the data.

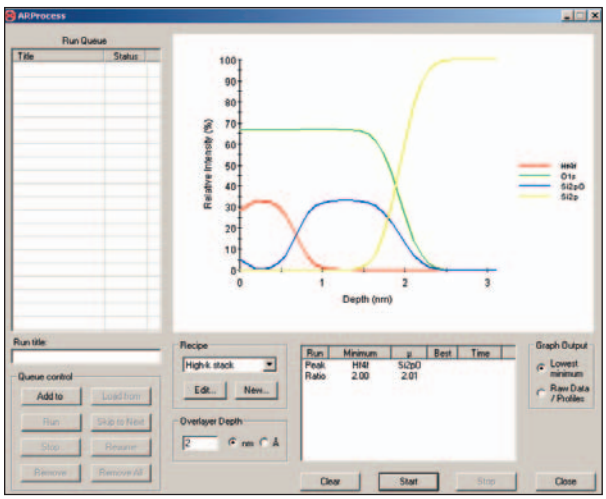

Figure 11: Construction of a depth profile from ARXPS data

As with the multiple overlayer calculator, the physical properties required to calculate the results are contained in a database. The user can edit the database values and define recipes for each type of sample.

If a large number of profiles need to be constructed, the user may place each data set in a queue so that they can be processed without further user intervention.

Multi-Dimensional Data Display

It is possible to perform many different types of surface analysis experiments and *Avantage* caters to them all. This gives rise to a large number of different variables which need to be displayed:

- Energy
- Intensity
- Peak area
- Time
- Depth
- Distance
- Direction in x and y
- Angle

In some experiments several of these need to be displayed simultaneously. For example, in an angle resolved XPS experiment energy, intensity and angle will need to be displayed simultaneously. For an image, x, y and intensity will need to be displayed. A montage display would be appropriate for the ARXPS case and a false color map may be better for the image. *Avantage* has a variety of different methods for displaying the data so that the best method can be chosen for each data set.

The type of display used for a given data set is totally under the control of the user. For example, if a set of spectra from a depth profile are plotted on a map with depth shown on one axis, energy on the other axis and color representing the intensity it is often possible to see intermediate chemical states more easily than if a montage were displayed.

To illustrate the versatility of the display options, Figure 12 to Figure 16 show the data from a depth profile (Al_2O_3 on Al) using 5 different display modes.

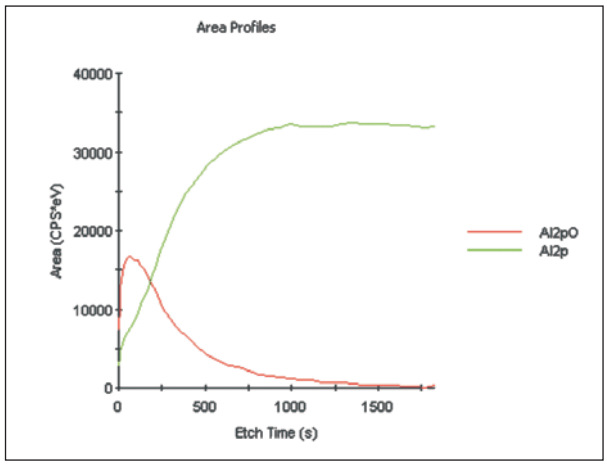

Figure 12: Graphical display of profile

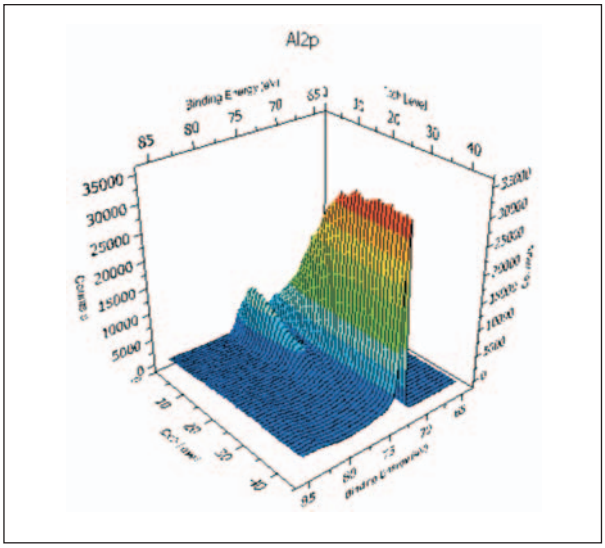

Figure 13: Montage display

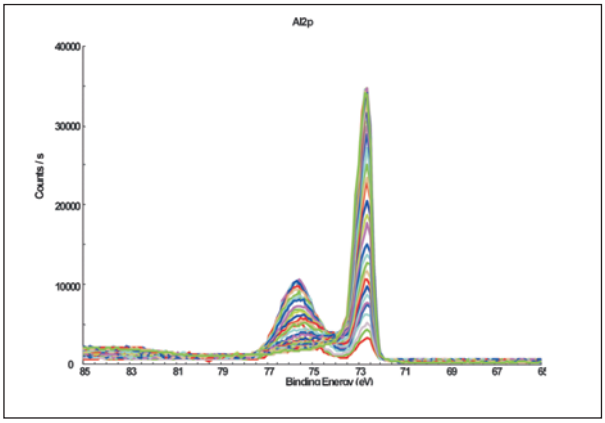

Figure 14: Comparison mode

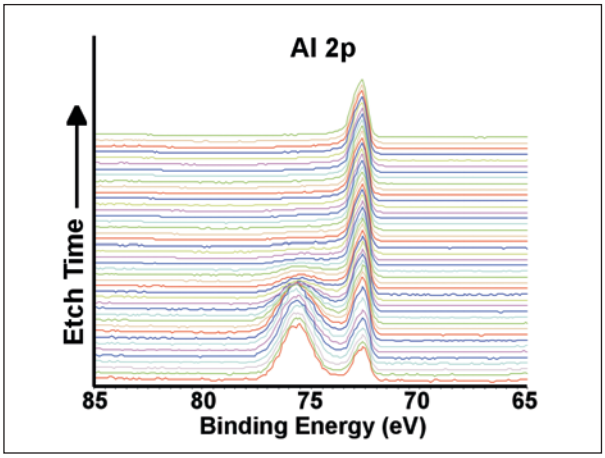

Figure 15: Stacked spectra

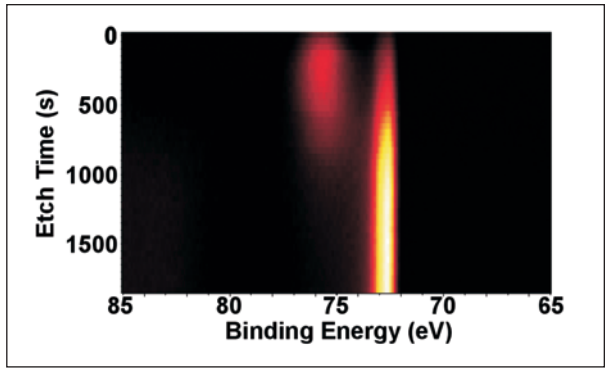

Figure 16: Image mode with energy represented in the x direction and depth in the y direction

Data Processing Tools Summary

Space does not permit a detailed description of all of the available data processing tools available with *Avantage*. However, there follows a list of the more important ones.

Data Output

- Data may be printed or copied to the Windows clipboard for pasting into other software packages as pictures or data
- Data within a processing document may be saved, together with intermediate stages of processing
- Processing operations are recorded in an audit trail with the data

Annotation

- Annotate image in user selectable fonts and styles

Spectrum Processing

Processing operations include:

- Spectrum analysis
- Spectrum modification
- Profile processing
- Overlay/Comparison
- Non-Linear Least Squares Fitting and Target Factor Analysis

Spectrum Analysis

- Find/Add peaks (manual/auto)
- Identify peaks (auto/manual by energy range or by element)
- Peak quantification table (atomic concentrations, peak area, normalized peak area, transmission function correction, sensitivity factor)
- Add, remove, edit peaks
- Libraries include Scofield (XPS), Wagner (XPS), Auger and user definable
- Copy peak table to Windows clipboard

Spectrum Modification Options

- Smooth: Savitzky-Golay, Gaussian or Fourier
- Background subtraction: Shirley, Linear, Tougaard
- Differentiation and Integration
- Charge shift correction by peak reference or by cursor
- Charge shift correct single/all regions/levels

Automatic Peak Fitting

- Peak fit with up to 26 peaks. (Simplex or Powell algorithm)
- Peak fit parameters; Peak centre, width, height, shape G/L ratio etc
- Asymmetric tail parameters (mix, exponential, height)
- Interactive; add/remove/modify/delete peaks
- Fix, link or constrain peak parameters
- Peak fit at every level

Profile

- Profile types include peak area, height, normalized area, atomic percentage, peak-to-peak height
- Multi-level processing; smooth/differentiate/charge correct prior to profile creation
- Interface width calculator
- X-axis as depth, time, distance, level etc.

Spectra Comparison/Overlay

- Overlay spectra, arithmetic operations, align, normalize spectra

Numerical Methods

- Non-linear and linear least squares fit, target factor analysis may be applied to multi-axis data including depth profiles, linescans and images. These fitting methods enable separation of overlapping elemental or chemical species

Image Display and Processing

Full range of display options, image annotation and processing retrospective extraction of point, line and area data

Image Display Options

- Grey/heat/cold color scales
- Interactively change contrast and brightness
- Display any pixel intensity
- Image overlay of 2 or 3 images
- Histogram display
- Display axes information

Image Processing

- Smooth with user editable filter
- Edge detection
- High/Low pass filters
- Erode, dilate, gradient
- Image arithmetic; Add, subtract, divide, multiply, image overlay

Retrospective Linescans and Spectrum Analysis

- Linescan between any user defined points, with user defined width
- Reconstruct spectra from defined areas of image

Scatter Graphs

- Generate scatter graph from any two images and reconstruct multiple images from any part of the scatter graph

www.thermo.com/surfaceanalysis

In addition to these offices, Thermo Fisher Scientific maintains a network of representative organizations throughout the world.

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