

Increased Throughput Using Snapshot Spectra

Key Words

- Surface Analysis
- Fast Acquisition
- Multi-channel Detection

Thermo Scientific Theta Probe has a 2-dimensional detector which allows up to 112 energy channels to be collected simultaneously with up to 96 angle channels. Thermo Scientific K-Alpha has a 128-channel detector.

When multi-channel detection is used for spectrum acquisition in a hemispherical analyzer, each detector is set to a different energy. The range of energies covered by the detector (ΔE_{Det}) depends upon the geometry of the analyzer and the pass energy (PE) to which it is set. A small PE results in a small ΔE_{Det} .

The large number of energy channels available in Theta Probe means that there are two possibilities for the collection of spectra:

- Scanned mode
- Snapshot mode

In scanned mode the energy setting of the analyzer changes with time during acquisition. In snapshot mode the whole of the required energy range is dispersed over the detector so the energy setting of the analyzer remains constant throughout the acquisition.

Scanned Mode

When operating in the scanned mode, all multi-detector XPS spectrometers must be “over-scanned” to ensure that each detector collects electrons from the entire energy range. Figure 1 illustrates this. The energy range for the required spectrum is $\Delta E_{\text{spectrum}}$ and the energy range of the detector is set to ΔE_{Det} . At the start of the scan, the detector which collects the highest kinetic energy must be set to the lowest kinetic energy required for the spectrum. As a result, the other detectors are collecting signal which will not contribute to the final spectrum. As the analyzer is scanned, more of the detector energy range contributes to the final spectrum. At the end of the acquisition, the scanning must continue until the detector set to the lowest kinetic energy reaches the highest energy required in the spectrum. Thus, in order to obtain a spectrum over the range $\Delta E_{\text{spectrum}}$ it is necessary to scan the analyzer by an amount $(\Delta E_{\text{spectrum}} + \Delta E_{\text{Det}})$. This means that the collection time for the experiment is increased by the ratio $(\Delta E_{\text{spectrum}} + \Delta E_{\text{Det}}) / \Delta E_{\text{spectrum}}$

In addition to the time penalties associated with over-scan, there are time overheads due to the scanning process (stepping and settling times) which also increase the acquisition time.

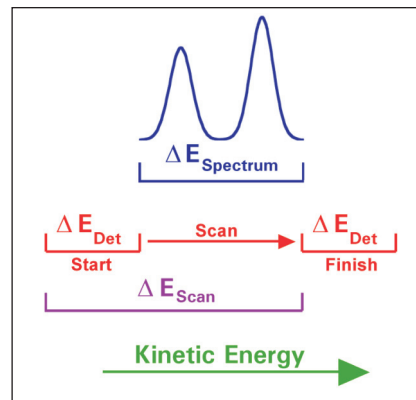


Figure 1: Acquisition of a scanned spectrum, showing the energy range of the detectors and the required scan range (ΔE_{Scan}) to produce a spectrum over the range $\Delta E_{\text{spectrum}}$

Snapshot Mode

In snapshot mode, the energy range of the detector is set to be equal to the required energy range for the spectrum (Figure 2). Electrons from the whole energy range are then collected simultaneously. The time penalties associated with over-scanning, stepping and settling are therefore eliminated.

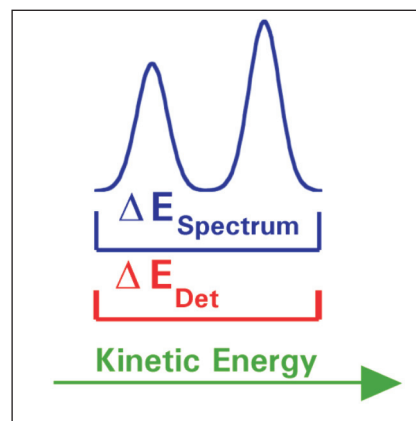


Figure 2: Acquisition of a snapshot spectrum, showing the energy range of the detectors throughout the acquisition

Comparison of Scanned and Snapshot Acquisition

The Ag 3d region of the XPS spectrum of pure silver was acquired in both scanned and snapshot modes using Theta Probe. In each mode of operation the PE was set to 100 eV. The scanned spectrum was taken and then the snapshot spectrum was collected until the Ag 3d_{5/2} peak was the same intensity as in the scanned spectrum.

The spectra are shown in Figures 3 and 4. As well as having the same intensity, these spectra contain the same number of energy channels (112). The peak width is the same in each case (FWHM = 0.95 eV) and the background signal is also the same.

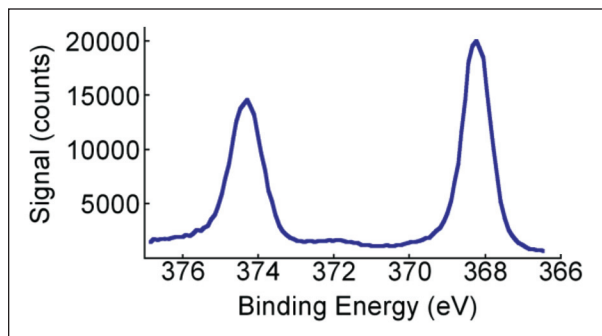


Figure 3: Scanned spectrum of the Ag 3d region of the silver XPS spectrum

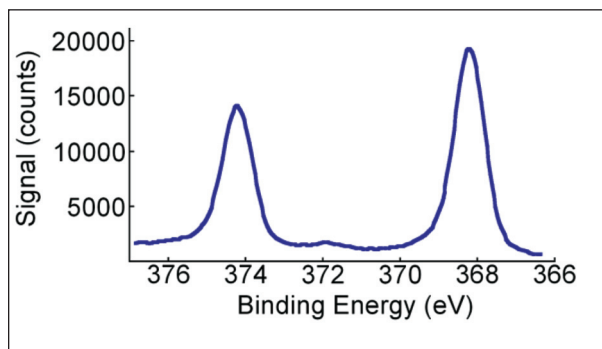


Figure 4: Snapshot spectrum of the Ag 3d region of the silver XPS spectrum

The only significant difference between these spectra is their acquisition time:

Scanned Spectrum acquired in 32.3 seconds

Snapshot Spectrum acquired in 11.3 seconds

Under these conditions, the snapshot spectrum was acquired in about one third of the time required for the scanned spectrum.

Whenever a spectrum is acquired in snapshot mode, the acquisition will always be faster than in the scanned mode because data is being collected during the whole acquisition period, there is no time penalty associated with over-scanning the spectrum.

The *Avantage* data system allows the user to select both the number of channels in the spectrum (up to 112) and the energy range in the snapshot. The pass energy is automatically set to produce the required energy range.

Major Time Savings Using Snapshot Spectra

Savings in the acquisition time can be achieved whenever the snapshot mode is used. This is particularly significant when large data sets are required. Typically, large data sets are needed for the following experiments and their combinations:

- Depth profiles
- Maps
- Angle resolved measurements
- Multi-point analysis
- Line scans

Quality of Snapshot Spectra

Snapshot spectra will be of high quality only if the detector has a large number of channels, as is the case in Theta Probe with its 112 channels.

Figure 5 shows a series snapshot spectra from oxidized tin. Each spectrum shown was collected with a different number of energy channels ranging from 8 to 112. Only when a large number of channels are collected (>56) is the quality of the data high enough to be useful.

High quality spectra are necessary to identify and quantify small chemical differences which may be present in the data set. This may be achieved by the application of Target Factor Analysis and Non-Linear Least Squares Fitting using *Avantage* data system.

Throughput

Sample throughput cannot be determined by counts per second alone. The most important factor is the time to complete the analysis. Snapshot capability significantly increases throughput without sacrificing analytical information.

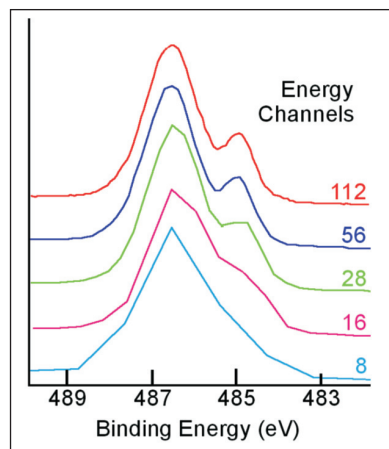


Figure 5: Spectra from a sample of oxidized tin showing how the quality of the snapshot spectra improves as the number of channels increases

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Africa
+43 1 333 5034 127

Australia
+61 2 8844 9500

Austria
+43 1 333 50340

Belgium
+32 2 482 30 30

Canada
+1 800 530 8447

China
+86 10 8419 3588

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+45 70 23 62 60

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Netherlands
+31 76 579 55 55

South Africa
+27 11 570 1840

Spain
+34 914 845 965

**Sweden/Norway/
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+46 8 556 468 00

Switzerland
+41 61 48784 00

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+44 1442 233555

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