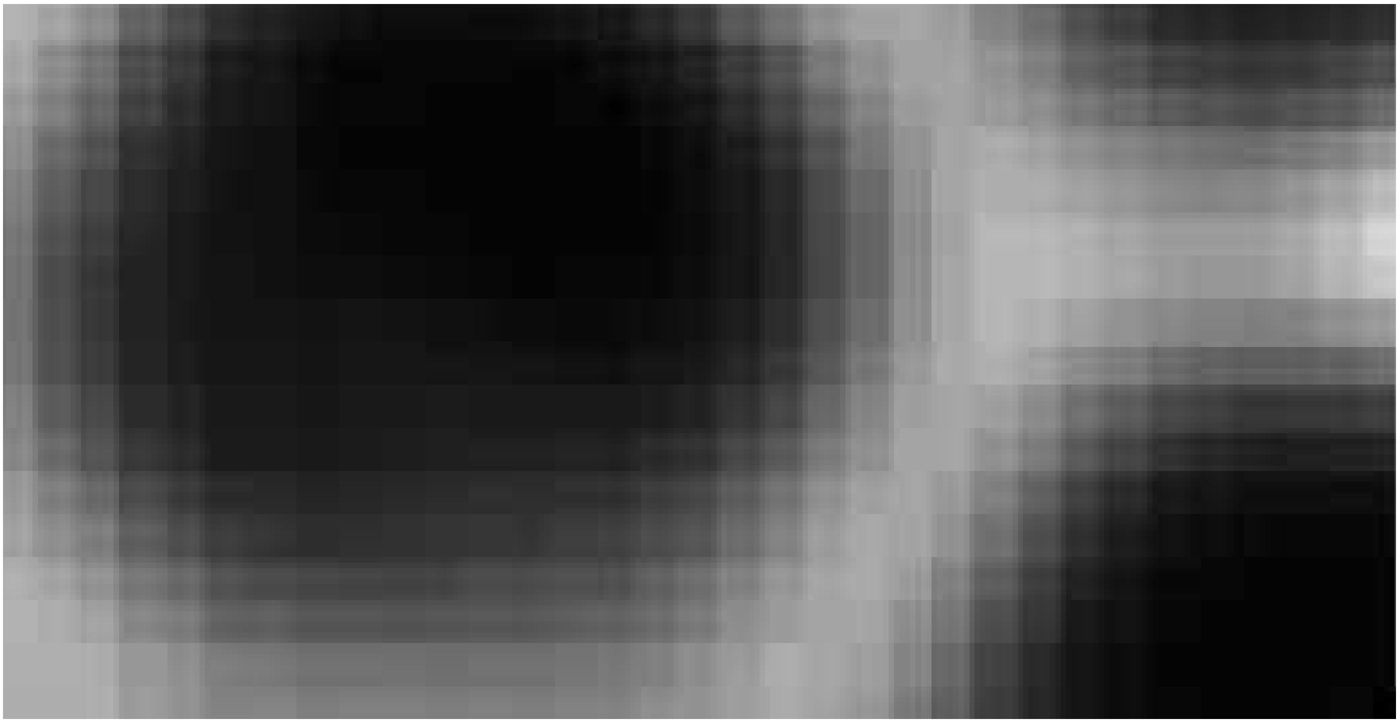
APPLICATION NOTE



Using Deconvolution Methods to Improve the Spectral and Spatial Resolution of XPS Data

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Thermo Scientific™ Avantage data system™ for surface analysis instruments has been enhanced by inclusion of new spectral and spatial deconvolution methods. These methods allow shorter data acquisition times, which can minimize X-ray degradation of the analyzed area. They can also improve the signal to noise ratio while maintaining the chemical state information from the sample.

Introduction

Chemical state information in XPS is maximized by using high energy resolution. Such analyses have reduced signal intensities so acquisition times are lengthened. On a modern spectrometer single point high-resolution spectra may be rapidly acquired, but spectrum accumulation time savings become very significant in multilevel acquisition such as depth profiling or imaging. Analysis time reductions are also important when analyzing polymers and organic samples since prolonged exposure to the X-ray probe may alter the chemistry of the surface.

New processing features based upon established spectral and imaging deconvolution algorithms have been incorporated into Thermo Scientific Avantage, the processing and control software for Thermo Scientific surface analysis instrumentation. Data can be acquired in a high sensitivity mode, by using a larger X-ray probe and/or more sensitive electron analyzer setting, and then deconvoluted to give the level of chemical state and spatial information usually associated with high energy resolution or smaller X-ray probe analyses. The benefits of higher sensitivity acquisition are maintained, i.e. shorter acquisition times and reduced exposure to the X-ray beam, without compromise to the ultimate data quality.

The mathematical basis of these techniques relies on removal of a point spread function from the data. A point spread function (PSF) describes the response of an imaging or spectroscopic system to a point source. The acquired data (in the XPS case, either a spectrum or an XPS image) is a convolution of the PSF for the measuring lens system and the intensity of each discrete point. This has been illustrated in the Figure 1.

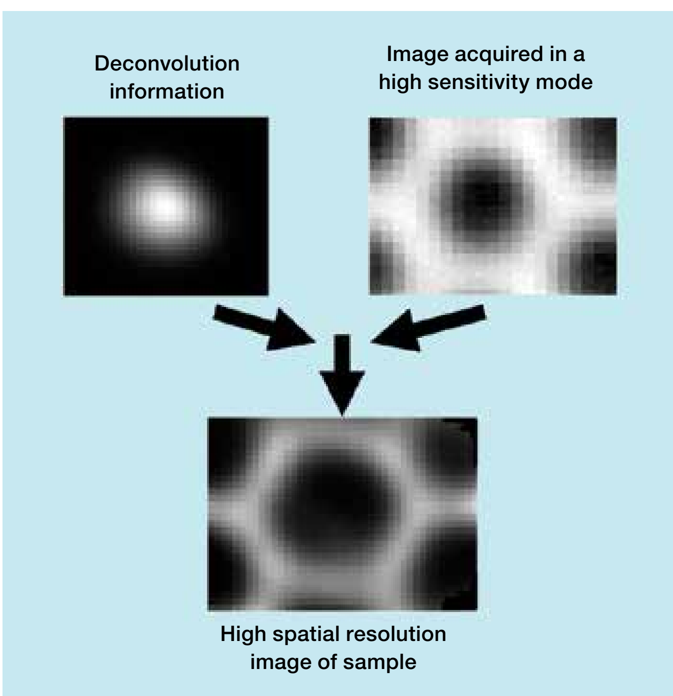

Figure 1: Using deconvolution information to recover spatial information from an image acquired in a high sensitivity mode

Experimental and Results

Two different algorithms have been used for the deconvo-lution routines depending on whether XPS image or spectra are in view. Both use an iterative approach which means that no prior knowledge of the data statistics is required, and the constraints and the boundaries can be easily incorporated to the algorithm.

Image Deconvolution

Image deconvolution is performed using an algorithm based on the Richardson-Lucy method.[1] It was originally developed and it has been proven useful with astronomical imaging and microscopy.

$$\hat{o}^{(k+1)}(x) = \hat{o}^{(k)}(x) \cdot s(-x) \times \frac{i(x)}{s \times \hat{o}^{(k)}}$$

This deconvolution method has now been adapted by Thermo Scientific for application to XPS imaging. The software automatically calculates the deconvolution information by measuring the intensity profile of the X-ray beam used for the image acquisition. The deconvolution function is then applied to each pixel of an image map to give the deconvoluted image. An example of image deconvolution, as implemented in the Avantage™ data system, is shown in Figure 2. By using this method the spatial resolution of an image can be brought towards the limit set by the stage step size which can be less than a third of the limit set by the X-ray spot.

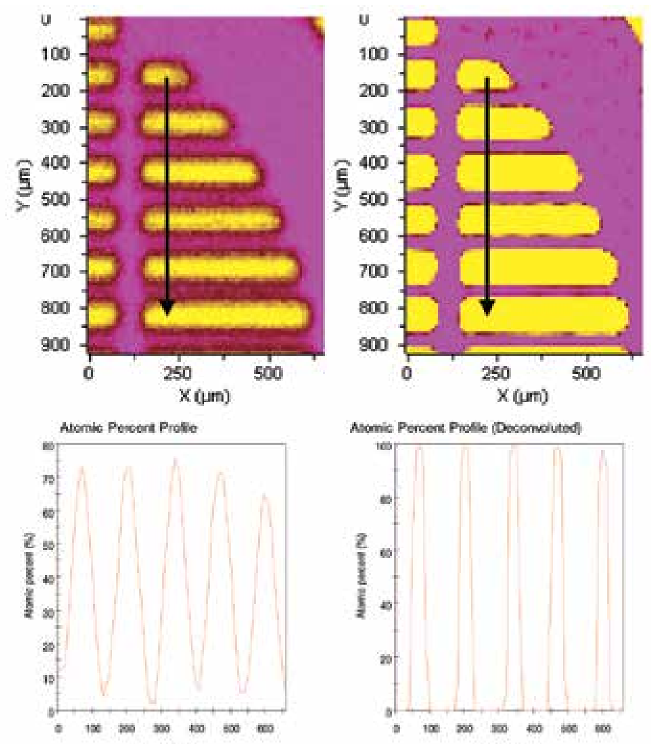

Figure 2: An example of using deconvolution information to recover spatial information from an image acquired in a high sensitivity mode. The image on the left is the original image and on the right after deconvolution. The linescans across the grids give the edge resolution of 30 µm for the original image (the same size as the X-ray spot size used). The average resolution for the deconvoluted image is 9 µm.

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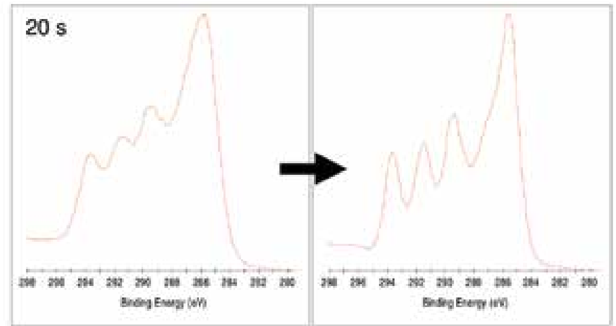
Spectral Deconvolution

For spectrum processing, the deconvolution information is derived from spectra acquired from a standard material (such as silver) at a range of electron analyzer settings. The deconvolution algorithm is based on Jansson's method:[1]

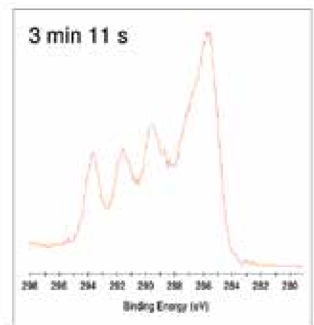
$$\hat{o}^{(k+1)} = \hat{o}^{(k)} + r\,[\hat{o}^{(k)}](i - s \times \hat{o}^{(k)})\hat{o}$$

A spectrum acquired in a rapid acquisition mode is shown in Figure 3a. (The total acquisition time was 20 s.) The spectral components are not well resolved, meaning that the chemical state information is obscured. Figure 3b shows the spectrum after deconvolution. The individual chemical state components are now easier to resolve and the overall good signal-to-noise ratio of the original spectrum is maintained. Data acquired in a higher energy resolution mode is shown for comparison (Figure 3c). (The total acquisition time for this data was 3 min 11 s.) The chemical state information which can be derived from the deconvoluted spectrum is equivalent to the level of chemical information in the spectrum acquired at high energy resolution, but the amount of time required to achieve this was ten times shorter. This is ideal for mapping and depth profiling applications where large numbers of spectra are being acquired, and for sensitive samples that could be damaged by prolonged exposure to the X-ray beam.



a) Rapid acquisition mode. Excellent S/N ratio

b) Deconvoluted spectrum. Excellent S/N ratio and resolution



c) High energy resolution mode

Figure 3: Using deconvolution information to recover chemical state information from a spectrum acquired in a high sensitivity mode

Summary

The new processing routines available in Thermo Scientific Avantage software have substantial benefits to offer to XPS sample analysis. Reductions in acquisition time are possible by using higher pass energies, resulting in lower exposure of sensitive samples to the X-ray source and multilevel data sets in particularly are acquired more rapidly. Extracting information from the data can be easier due to improved signal-to-noise ratios and image deconvolution takes us beyond the already excellent spatial resolution.

Keywords
Avantage, Chemical Imaging, Deconvolution, Surface Analysis, XPS

Reference

1. Deconvolution of Spectra & Images (2nd Ed), Peter A Jansson (Ed),Academic Press (1996)

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