AES Features in CasaXPS

Converting AES Direct Spectra to Differential Form

Spectra acquired in direct form must be processed into the differential format before proceeding to quantification. The steps to convert an entire data-set to differential format are as follows:

1. Select a spectrum into the Active Tile.
2. Enable the Processing menu/toolbar option by left-clicking the Active Tile, then invoke the Spectrum Processing dialog window using the Processing option on the **Options** menu.
3. Using the Differentiation property page on the Spectrum Processing dialog window, apply a five point Savitzky-Golay, quadratic polynomial differentiation to the data (Figure 1).
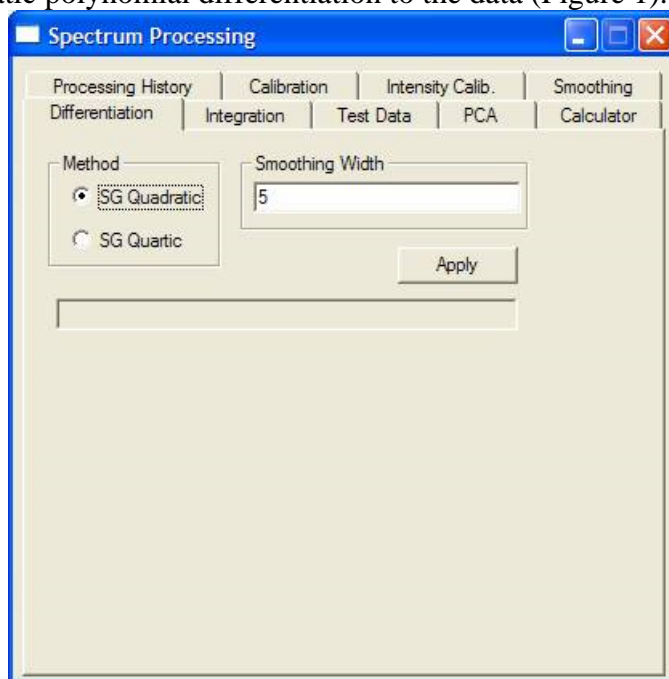

Figure 1

1. Select all the VAMAS blocks in the right-side browser and propagate the processing to all the selected spectra.
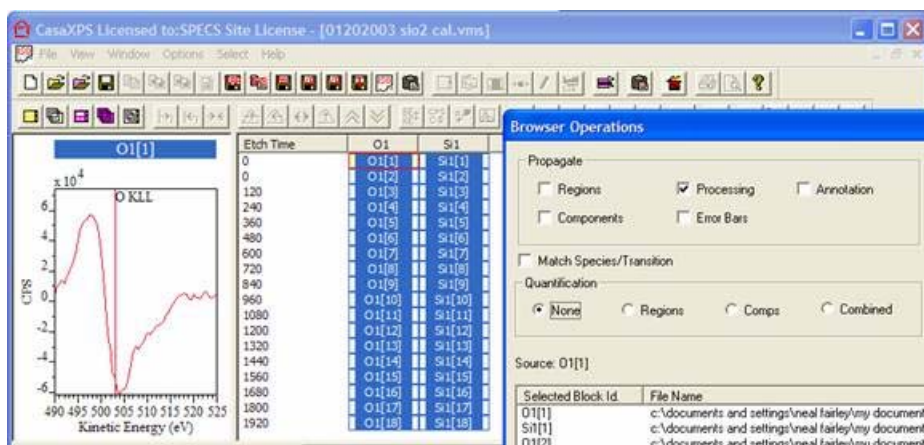

Figure 2

by Neal Fairley

Linear Least Squares Analysis of Chemical States

Chemical State information within AES differential spectra can be separated using linear-least squares (LLS) provided representative spectra are available for the desired chemical states. The LLS option is available on the PCA property page on the Spectrum Processing dialog window (Figure 3). In the example shown in Figure 3, two states have been selected to represent the Oxide and Metallic Si signal and are displayed in the Active Tile. These two spectra in the Active Tile represent the basis set used as part of the LLS procedure, while the set of data selected in the right-hand-side of the Experiment Frame are the unknown data to be analysed by LLS. That is to say, when the button, labelled Generate Spectra on the PCA property page shown in Figure 3, is pressed the appropriate linear combinations of the two spectra in the Active Tile are determined for each of the spectra selected in the right-hand-side and a new Experiment Frame is created. The contents of the new Experiment Frame are: the original spectra, a spectrum computed from the linear combination and the scaled basis spectra determined from the LLS calculation. Assuming the LLS can property account for the states within the unknown spectra, the scaled basis spectra can be used to quantify the relative proportions of the known chemical states. It will be necessary to move the scaled basis spectra into the same Experiment Frame as any other spectra also part of the analysis, such as the oxygen region also shown in Figure 3. Quantification can then proceed as described below.
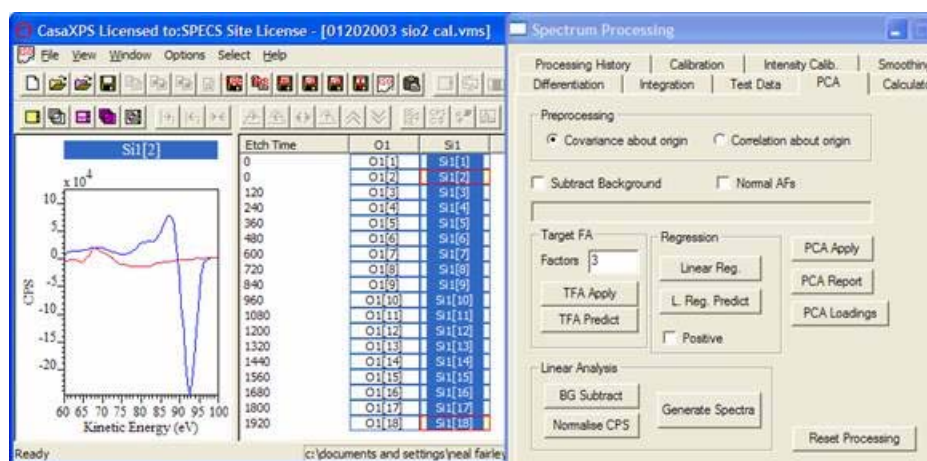

Figure 3

Quantifying Spectra Using Peak-to-Peak

Quantification of AES differential spectra is typically performed using peak-to-peak intensities. The Regions property page on the Quantification Parameters dialog window Figure 4) displays both the maximum/minimum intensities within a region and also the Peak-to-Peak atomic concentration (although the term **atomic concentration** only applies when an elemental analysis is performed on a survey spectrum). The background type is irrelevant to the computation of these intensities, provide a background can be computed, however from an aesthetic point of view a choice of mean or zero background types would be appropriate.

Quantification for sets of narrow scan data is achieved using the Report Spec property page on the Quantification Parameters dialog window. The Standard Report can be customized to display only the Peak-to-Peak concentration results, while the, so called, Custom Report interface offers a button for generating a profile using peak-to-peak intensities. The essential mechanisms described elsewhere for XPS spectra also apply to AES quantification.
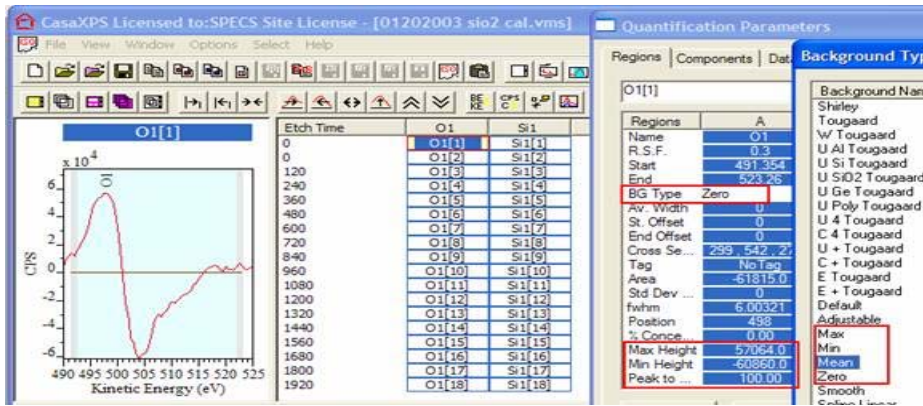
Figure 4

Quantification: An Example

In this example, an AES depth profile acquired using the RBD Auger Scan software is analysed using LLS to separate metallic Si from Si oxide. The profile is generated from quantification items defined on each of the LLS components together with the oxygen spectra. Figure 5 shows the direct spectra before any processing is applied.
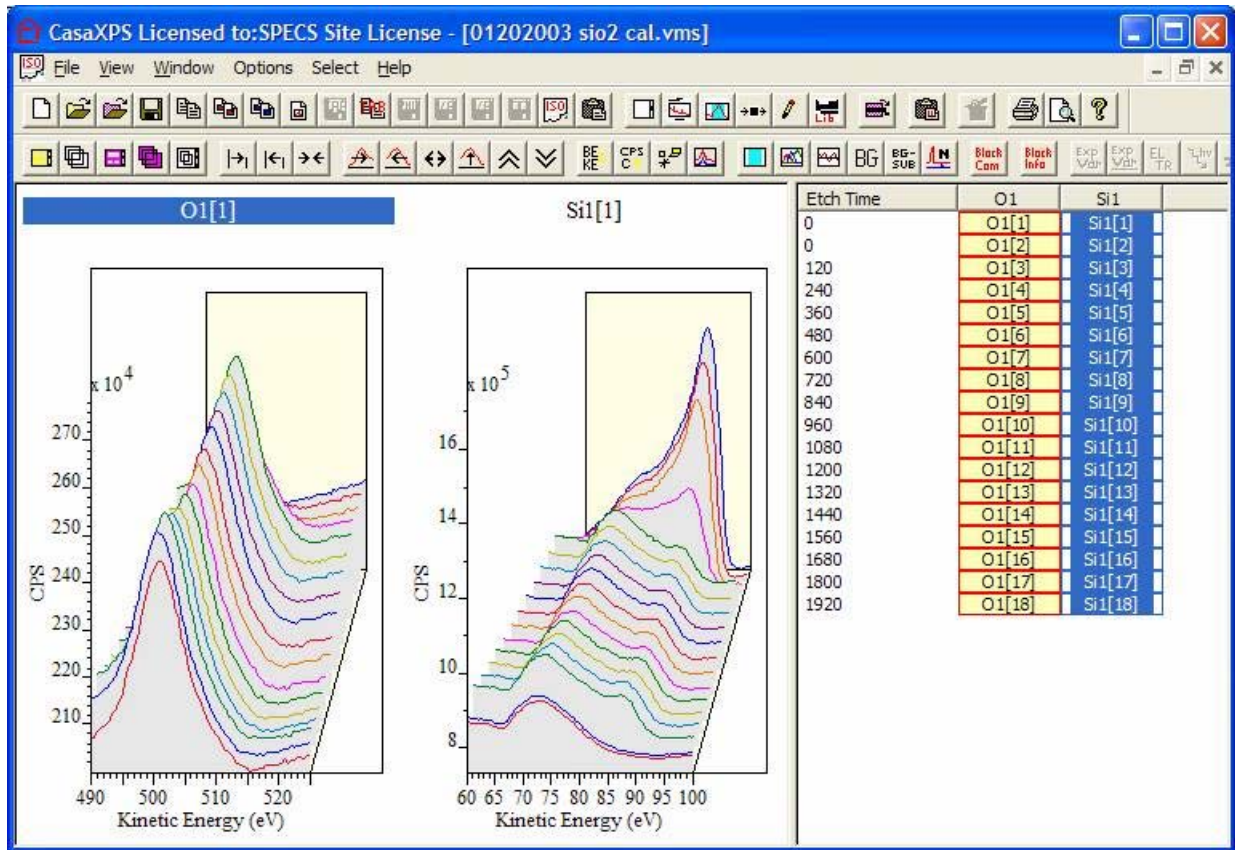

Figure 5

Step 1: Differentiate Spectra

AES spectra are typically quantified using peak-to-peak intensities taken from the differential of the direct

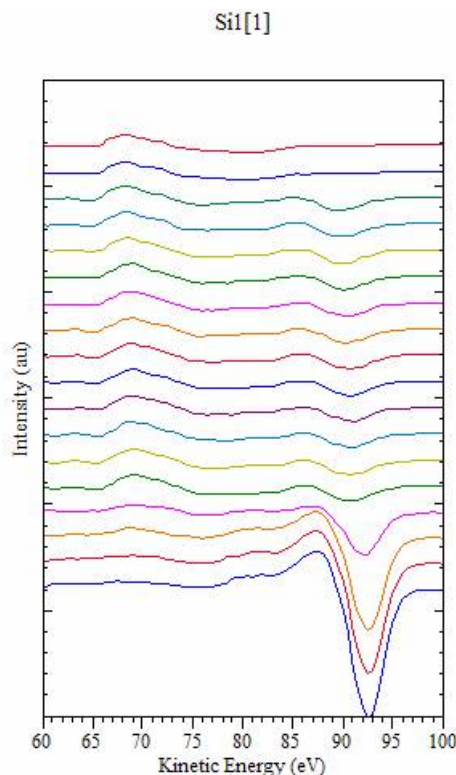spectra. The spectra must be all converted to differential form using <u>the procedure described above</u>.

Figure 6

Step 2: Separate the Metal and Oxide Silicon States

A <u>LLS procedure</u> using three basis spectra taken from the profile provides the means for estimating the contributions from the metal and oxide present in the silicon spectra. A representative set of spectra after the LLS has been applied in shown in Figure7. The three basis spectra scaled by the LLS procedure are displayed in the second column labelled Surface Si, Si in SiO2 Layer and Si Metallic. Combining these three scaled Si spectra results in the blue trace in the top left-hand tile, while the red trace is the original spectrum modelled by the blue trace.

Note, the O1 spectra have been copied into the Experiment Frame created when the LLS procedure was applied to the Si spectra. This allows quantification regions to be assigned to each of the Si basis spectra and also the O1 data. The profile shown in Figure 8 is the result of quantifying the entire data set using the Height Report from the Custom Report section of the Report Spec property page on the Quantification Parameters Dialog Window.
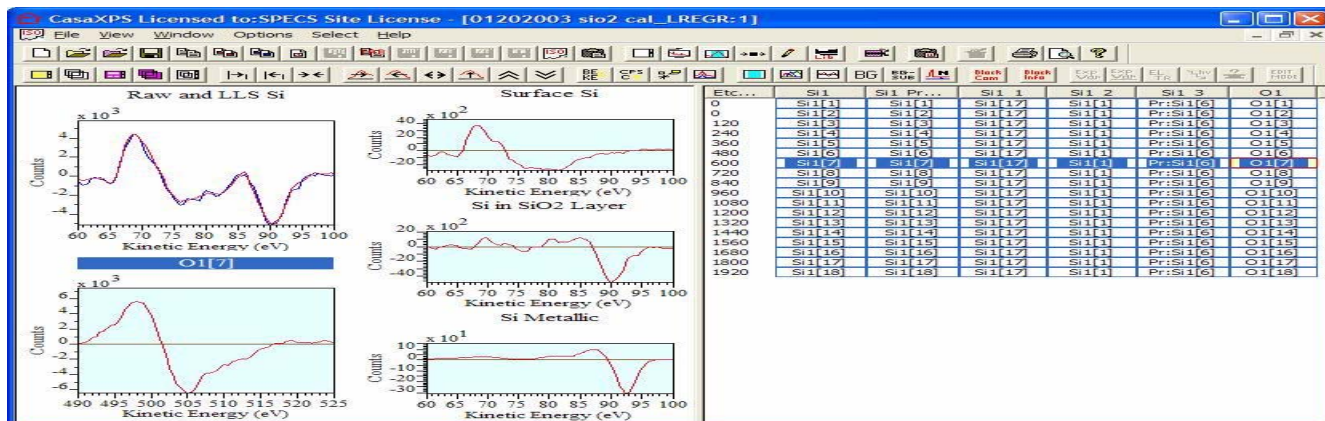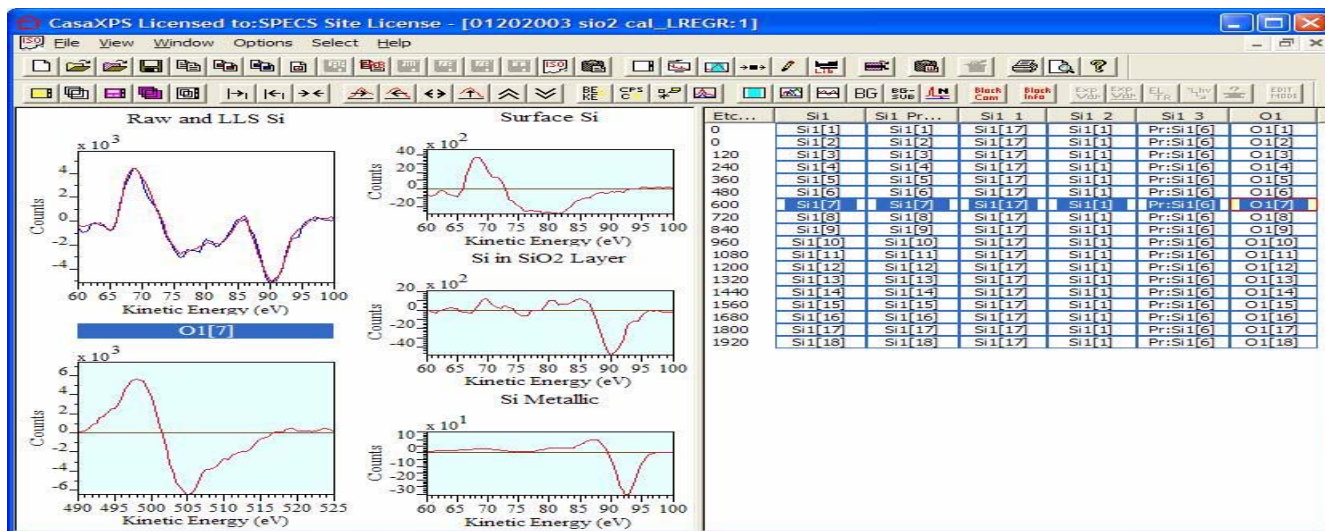
Figure 7

Three basis spectra were used in the LLS, one taken from the surface regions, one taken from the metallic region and the third created from a Si spectrum within the oxide layer after first subtracting the surface spectrum. Such a procedure is necessary, from a numerical perspective, to allow reasonable accuracy between the raw Si spectra and the reconstructed spectra. The trace labelled "Si?" in Figure 8 could be viewed as part of the metallic signal and therefore these two intensities could be summed using the Custom Report (Figure 9). The result of creating a Height Report using the definition shown in Figure 9 is offered in Figure 10.
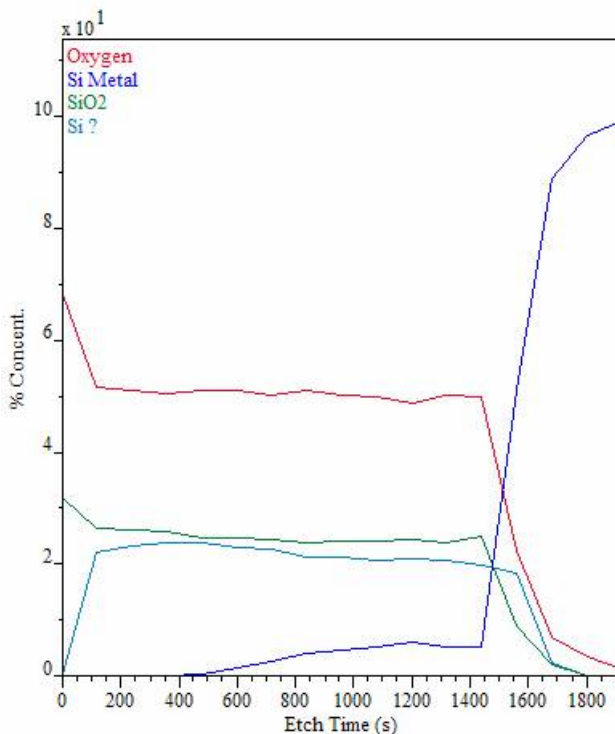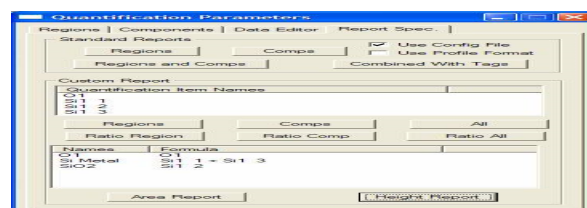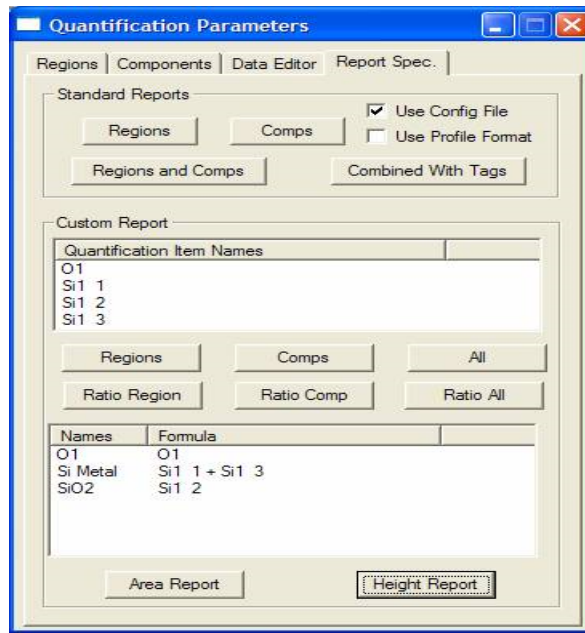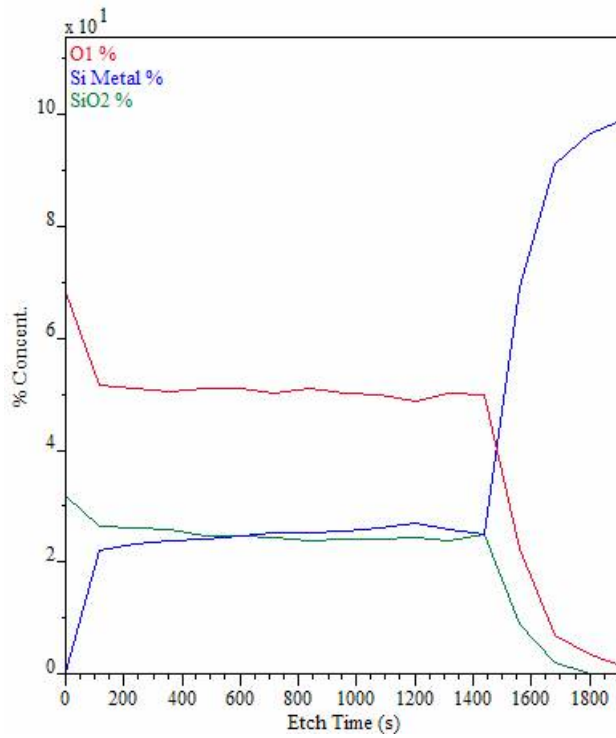

Figure 8

Figure 9

Figure 10