

## **Visualising Spectra**

A common requirement is to display spectra from a sequence of experiments in an overlay plot where the intension is to visually inspect the variation in the data with respect to the changing experimental conditions. The data in Figure 1 are a sequence of measurements from a silicon sample acquired at different angles of sample tilt. The spectra vary as a consequence of the depth sampled by the analyser with each change in the angle. The raw data for five angles are shown in Figure 1.



Raw Data No Scaling

Figure 1: Raw Data

The display in Figure 1 shows the relative intensities of the elemental and oxide peaks varying with angle, however the counts per second (CPS) also reduces with angle. One solution often employed to remove the reduction in CPS is to normalise with respect to the area of the region defining the Si 2p peaks. The consequence of normalising to the peak area, as seen in the right-hand-side of Figure 2, is that the peaks are scaled to provide a uniform appearance and size. While permitting the data to be plotted on the same axis scale, the relative importance of the peak sizes to the sample composition is as misleading as the plot in Figure 1. As an alternative to the normalisation offered on the Calculator property page, a further means of scaling the data is offered on the Test Data



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property page of the Spectrum Processing dialog window. The *Quant Scale* button on the Test Data property page provides a scaling equivalent to the results obtained from a quantification report. That is to say, the peaks are background subtracted and then scaled based on the total CPSeV adjusted for RSF and transmission corrections. The left-hand-side of Figure 2 plots the same data in Figure 1, where the peaks have been normalised with respect to both the intensity of the Si 2p peaks plotted in Figures 1 and 2 and also the corresponding set of O 1s data. The data are therefore visualised with the scaling used to generate quantification reports from regions; a procedure widely accepted as the correct means of comparing XPS data in tabulated format.



**Figure 2: Scaled Data** 

To prepare the data in the format shown in the left-hand-side of Figure 2, each spectrum used in the calculation must have at least one quantification region defined and the VAMAS blocks selected appropriately. The VAMAS blocks must be selected as shown in Figure 3, that is, exactly the same selection used to prepare a quantification report via the Report Spec property page. The **Quant Scale** button (Figure 4), when pressed, causes the spectra to be background subtracted and scaled with respect to the total intensity from the Si 2p and the O 1s spectra, one row at a time as shown in Figure 3.



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	Angle	Si2p	Si2s	O1s		
	90	Si2p 1	Si2s 13	O1s 25		
	70	Si2p 2	Si2s 14	O1s 26		
	50	Si2p 3	Si2s 15	O1s 27		
	30	Si2p 4	Si2s 16	O1s 28		
	15	Si2p 5	Si2s 17	O1s 29		
	25	Si2n 6	Si2s 18	O 1s 30		



Spectrum Processing					
Processing History Calibration Intensity Differentiation Integration Test Data	Calib. Smoothing PCA Calculator				
Generate Test Data PMMA PMMA + Shirley	Gain/Offset				
PVA PVA + Shirley	0				
PVC PVC + Shirley	0				
Image Spectra	0				
Replace By Envelope Add Noise Sum	Apply				
Background Subtract Merge Sum All	Write ASCII				
Create Spectrum From Components Fix Image Set Value					
Create SPECSLAB I TRF (Data - Bg) / Bg Quant Scale					

Figure 4: Test Data property page including the Quant Scale.