

Charge Correction for iXPS

An iXPS data set consists of a spectrum at every pixel in an image. These spectroscopic image data sets may exhibit lateral differential charging as a consequence of:

- An uneven X-ray flux
- Different intensity of photoelectron emission across the field of view

This is not necessarily a problem for quantification where the limits of integration can be adjusted to accommodate the charging. Neither is it a problem for peak fitting where peaks can be fixed with respect to the primary peak which can be allowed to move within limits. However it is a problem for Principal Component Analysis (PCA) which is used to improve the signal/noise in the iXPS data set. PCA recognises different charge shifts as a separate component increasing the number of components and therefore the possibility that some will be lost in the noise of the data. Correction of charging at every pixel is therefore necessary. This page illustrates the steps required to do this.

The Sample

Islands of silicon oxide, approximately 150 nm high, were created on silicon by thermal oxidation followed by HF etching through a lithographic mask.

The Data

600 images of 256 x 256 pixels incremented in 1 eV steps from 600 eV to 0 eV were acquired over a 800 μm field of view, at 160 eV pass energy with a dwell time of 100 seconds. The raw O 1s, C 1s and Si 2p images are shown in figure 1. The images are converted to spectra, shown in figure 2, but the signal/noise is not sufficient to allow accurate determination of the C 1s peak position.

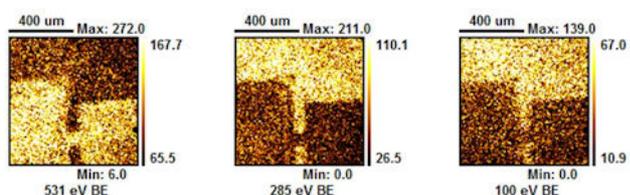


Figure 1. O 1s, C 1s and Si 2p raw images

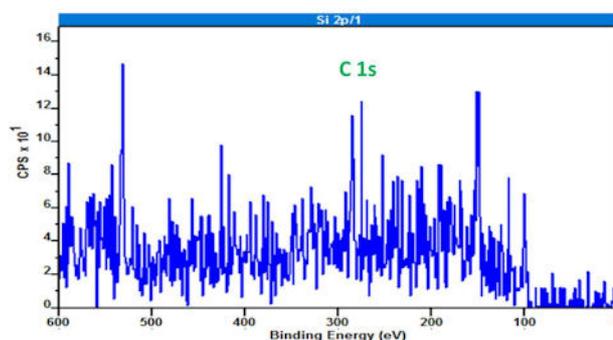


Figure 2. Raw spectrum at a single pixel

The signal/noise must therefore be improved using PCA. The images are overlaid and the first 10 components calculated, and the data then reconstructed using only the significant components, in this case 6, following optimum scaling. This is accomplished by entering '10' in the 'No scans' field, '6'

in the 'No AFs' field followed by clicking the 'Pred OpS' button. When the PCA has finished, the images are converted to spectra by clicking the 'Convert Images to Spectra' button. The appropriate regions are highlighted in red in figure 3.

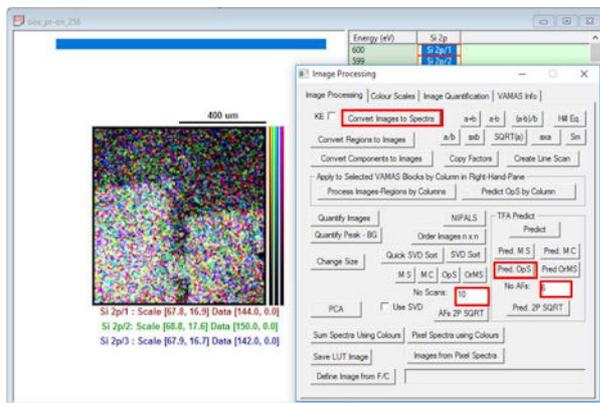


Figure 3. PCA data reconstruction using the first 6 components after calculating 12 using optimal scaling.

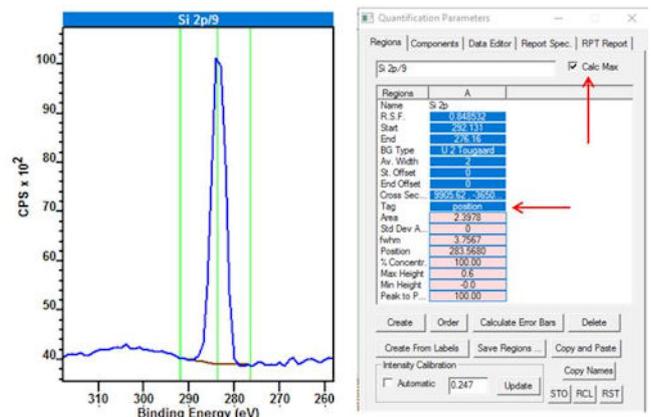


Figure 4. Determining the C 1s peak position

Once the images have been converted to spectra the C 1s peak position can be determined. The 'Quantification Parameters' window is opened and a region is defined around the C 1s photoelectron peak. The 'Calc Max' box is checked so that the peak position will be interpolated, and 'position' entered in the 'Tag' field, as shown in figure 4. This region is copied to all the other spectra by selecting their corresponding VAMAS blocks, and right clicking in the display pane to open the 'Browser Action' window, as shown in figure 5.

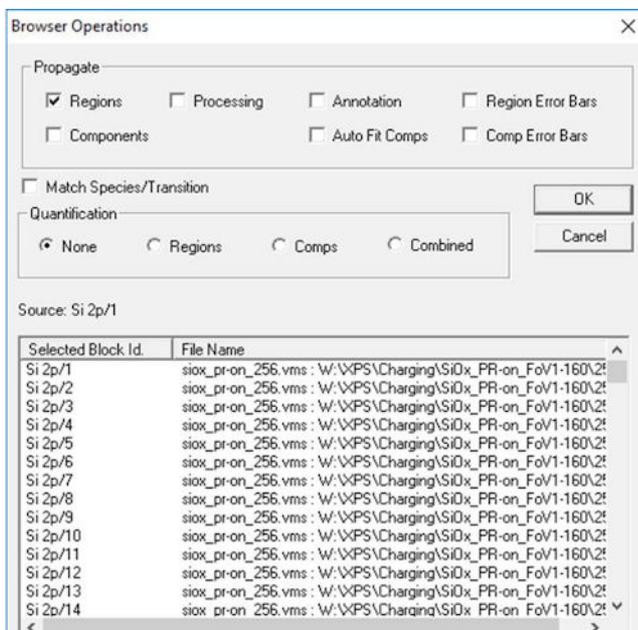


Figure 5. Copy the region to all spectra using the 'Browser Actions' window.

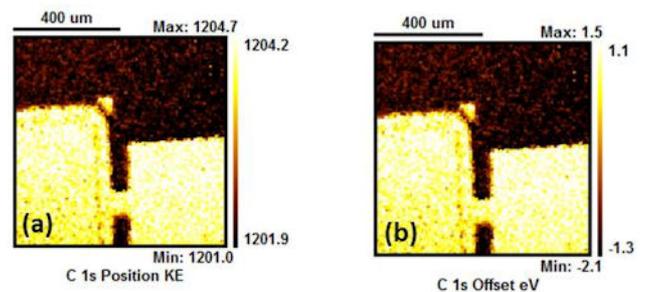


Figure 6. The peak position image (a), and the charge offset image (b).

Tick the 'Regions' checkbox, and press OK to copy the region properties to all the spectra listed. Select all the spectra and overlay them in the display pane. Clicking the 'Convert Regions to Images' button, seen in the image processing tab of the image processing window displayed in figure 3 computes an image consisting of the C 1s peak position of each spectrum in kinetic energy, shown in figure 6 (a). It is interesting to note that the thick oxide has a higher kinetic energy that is lower binding energy, than the native oxide, implying that the thick oxide is charging less. The 'Calculated Image StDev' highlighted in blue is used to calculate the mean, standard deviation, maximum and minimum values of the C 1s peak position. The charge offset image shown in figure 6 (b) is calculated by subtracting the mean value from figure 6 (a). This is accomplished by clicking the 'Image Calculator' button, highlighted in green, and entering the following string 'vb0 - [mean value]'. The reference is chosen as the mean value and not 285.0 eV, the value usually given to the C 1s hydrocarbon peak, because in a three dimensional data set each spectrum must be shifted, since the energy scale is common to all spectra and images will be lost as the spectra are shifted. The charge offset image is then copied to the raw data and displayed in the active window, as shown in figure 8. The images to be corrected are highlighted and the 'Charge Correct Images' button highlighted in red in figure 7 clicked. If more than one region requires correction they must be corrected separately so that images from one region are not transferred into a different region.

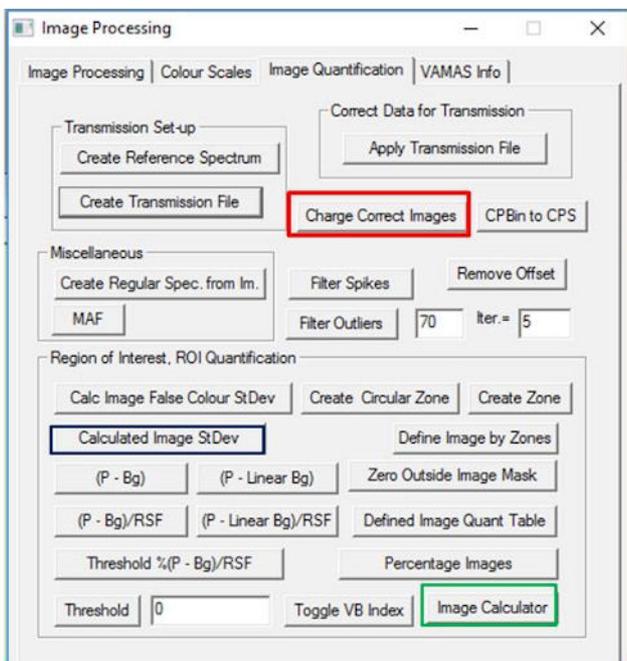


Figure 7. The Image Quantification Tab of the Image Processing window.

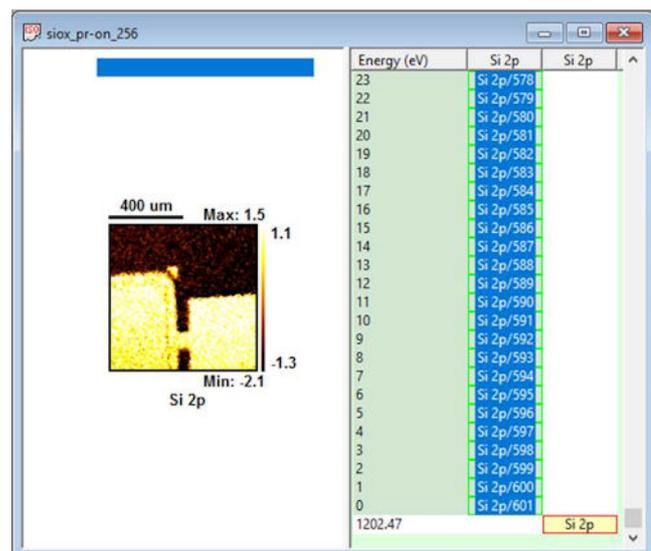


Figure 8. Applying the charge correction to raw images.

Figure 9 shows regions in the images containing zero counts as spectra have been shifted. These images must be deleted from the data set, and the maximum and minimum values of kinetic energy calculated with the image standard deviation can help. The charge corrected data set should now be saved. PCA should be carried out again to improve the signal/noise in the charge corrected data set, following which further processing such as quantification or peak fitting may be undertaken.

To illustrate the effectiveness of the charge correction procedure the pixels in the second image principal component have been classified by intensity into 16 segments and the spectra in each classification summed. Spectra from the raw data and charge corrected data are shown figure 10 (a) and (b) respectively.

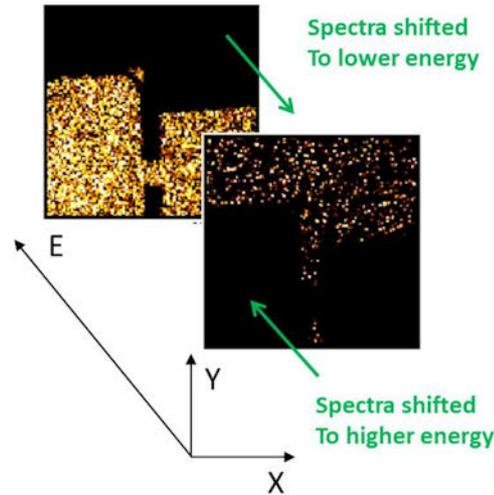


Figure 9. Loss of data at the end of the region caused by shifting the spectra

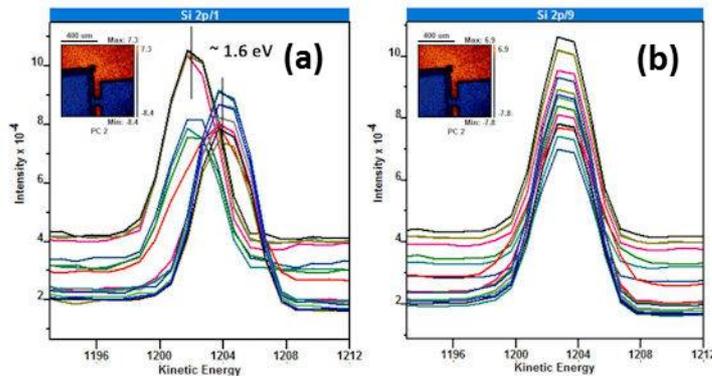


Figure 10 Spectra from the inset classification showing charging (a) and charge corrected (b).

Figure 11 shows the first six image principal components from the raw data, top, and from the charge corrected data, lower. There is clearly more information present following charge correction. The loss of information from the raw data is a consequence of charging resulting in more components which are unable to be effectively separated from the noise.

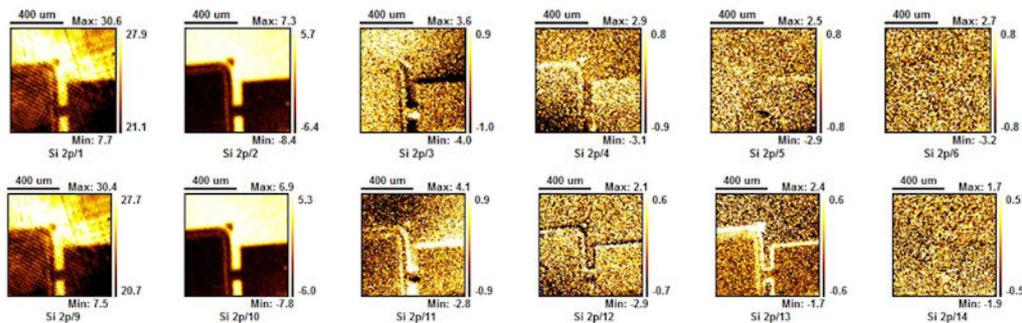


Figure 11. First 6 principal components from raw data (top), and charge corrected data (lower).

Figure 12 shows the carbon, oxygen and silicon atomic concentration images, calculated from the photoelectron peak areas following correction for the intensity/energy response of the instrument, and using Scofield sensitivity factors. The images are plotted from zero

intensity so as not to show any misleading contrast. There is a higher carbon concentration on the thermal oxide than the silicon/native oxide surface, which most likely arises from remnants of the photolithographic mask.

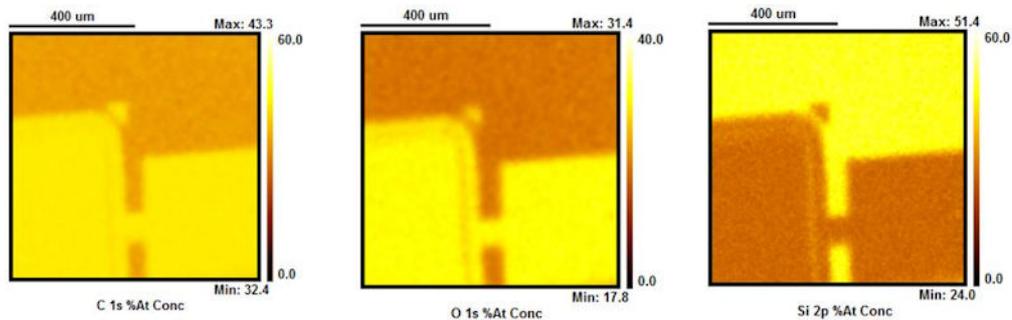


Figure 12. Atomic concentration images.

Figure 13 shows an overlay of the carbon and oxygen concentration images, which reveals a line of carbon surrounding the thermal oxide, consistent with the contrast seen in the higher order image principal components. This arises from emission of C 1s photoelectrons from the side wall of the thermal oxide. The line scan across the edge of the thermal oxide shows the carbon extends 12 μm past the edge of the oxide, which is consistent with the expected spatial resolution of the instrument at this field of view, and which couldn't be clearly observed without charge correction of the spectroscopic image data set.

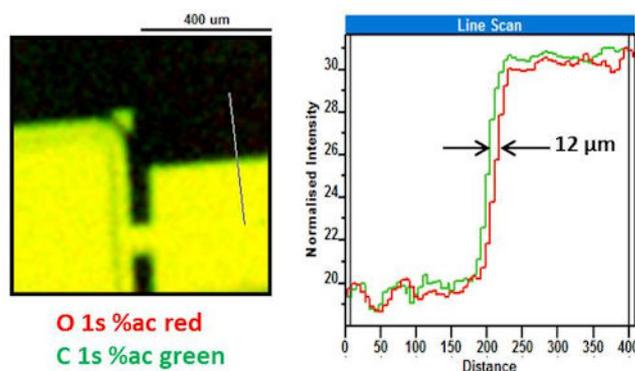


Figure 13. Overlay of O1s and C 1s atomic concentration images and linescan