

Chemical State Imaging with PHI Scanning XPS Microprobes

Overview: Compositional XPS images based on spectra obtained at each image pixel have been an important capability of PHI's scanning XPS microprobes since their introduction in 1995. These spectra provide peak area information used for 2D visualization of elemental distributions and quantification of XPS images. These spectra are also available for retrospective processing to search the image data set for variation in chemistry across the image and to create chemical state images. The spectra are collected at high speed using a multi-channel detector to capture a single element spectrum in one event. This data collection mode is commonly referred to as the unscanned or snapshot detection mode. To enhance this mode PHI has recently added the capability to collect unscanned spectra with up to 128 data channels on both the *VersaProbe II* and *Quantera II* scanning XPS microprobes.

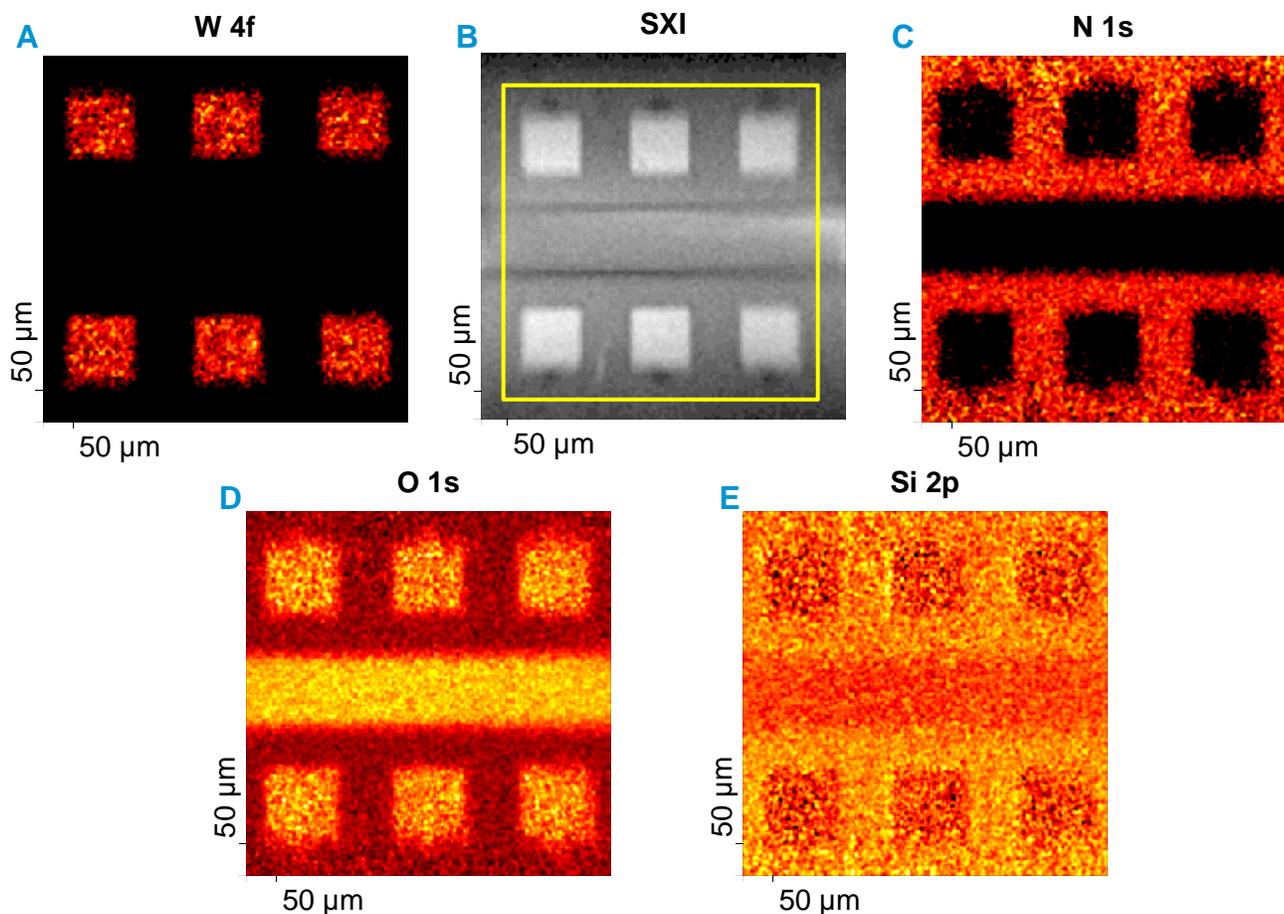


Figure 1. Panel B shows a Scanning X-ray Induced secondary electron image (SXI), from a cluster of bond pads on a semiconductor device structure, that was acquired in 30 seconds with a 500 μm field of view. Panels A, C, D and E show W 4f, N 1s, O 1s and Si 2p elemental intensity images respectively, from the area indicated in yellow in Panel B. At each pixel of the elemental images in panels A, C, D and E a spectrum with 128 data channels was obtained and the resulting peak area intensities formed the images.

Imaging Measurements: The semiconductor device structure was analyzed in the as-received condition with a PHI *Quantera II* scanning XPS microprobe. The x-ray beam diameter was set to 7.5 μm and dual beam charge neutralization was activated. The sample was placed at the focal point of the spectrometer using the instruments Auto-Z function and an x-ray beam induced secondary electron image (SXI) was obtained. As shown in panel B of figures 1 and 2 the area to be imaged was defined on the SXI image and is outlined in yellow. Because the secondary electrons are created and detected by the same x-ray source and energy analyzer used to acquire the XPS images, there is a perfect registry between the SXI images and the elemental images. The W 4f, N 1s, O 1s and Si 2p elemental images are shown in Figure 1; panels A, C, D, and E respectively. The data collection time for each image was 8 minutes. Each elemental image contains 256 by 256 pixels with each pixel containing a spectrum with 128 data channels. The elemental images in Figure 1 are XPS total peak area images. The bond pad structures which are approximately 100 x 100 μm are clearly visible in these images. These images contain spectra at each pixel with 128 data channels and the composite (spectra from all pixels added together) spectrum for each element is shown in figure 2. The arrays of spectra used to create the elemental images were then used with the Linear Least Squares (LLS) fitting algorithm in PHI MultiPak™ to create the chemical state images shown in figure 3.

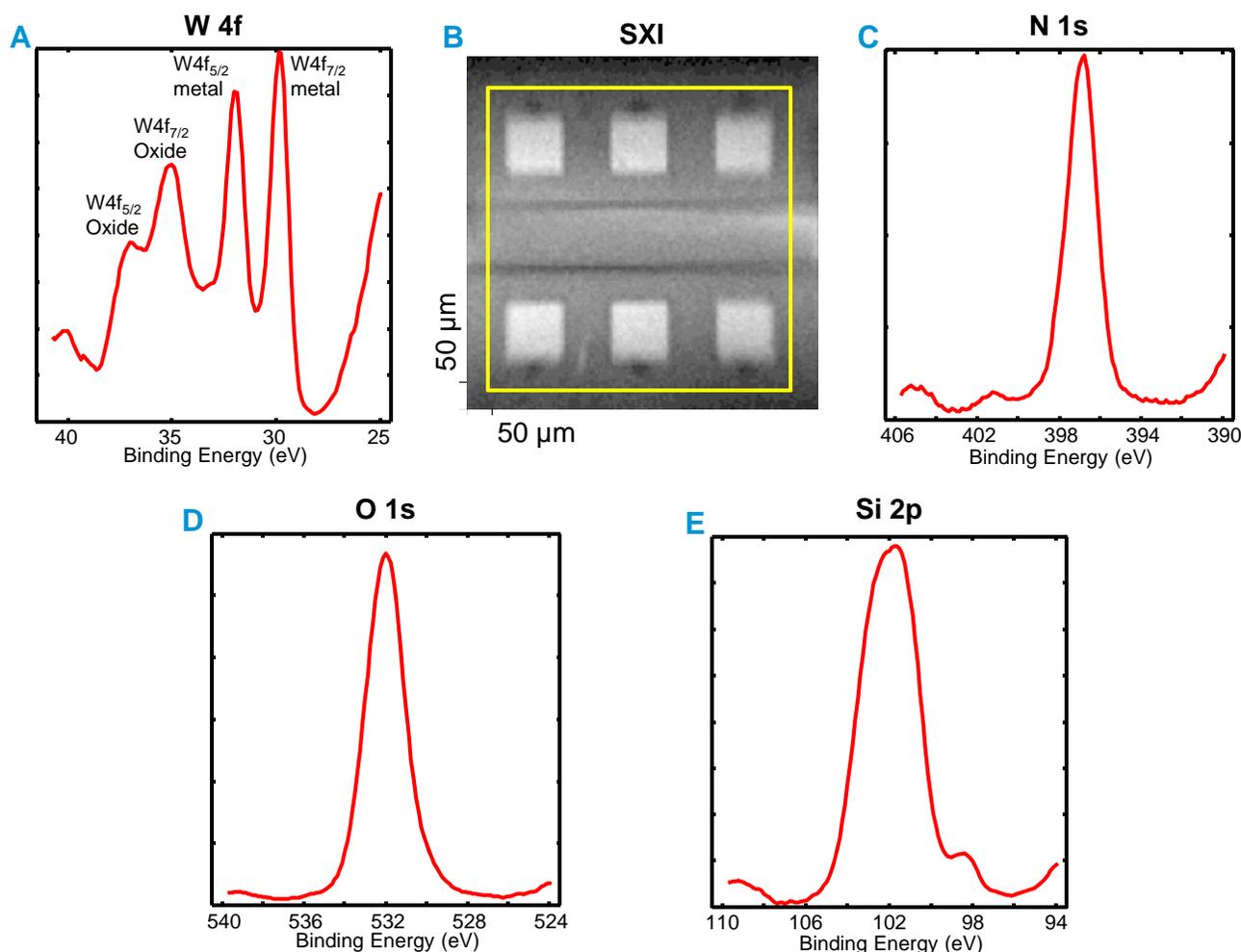


Figure 2. Panel B shows the Scanning X-ray Induced secondary electron image (SXI), from a cluster of bond pads on a semiconductor device structure, that was acquired in 30 seconds with a 500 μm field of view. Panels A, C, D and E show the composite spectra of W 4f, N 1s, O 1s and Si 2p resulting from summing the 128 channel spectra from all the image pixels.

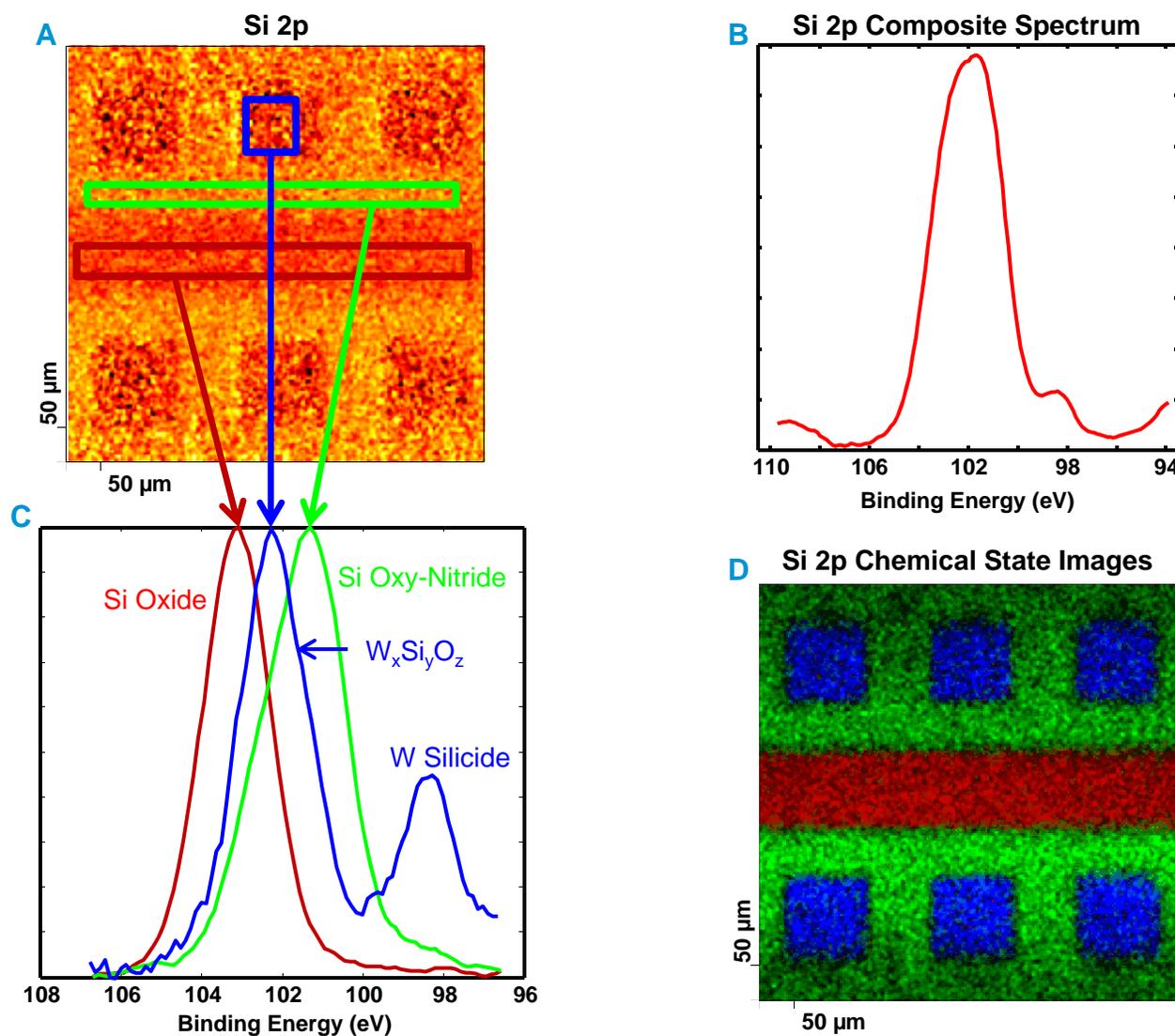


Figure 3. Panel A shows the elemental Si 2p peak area intensity image with three regions of interest selected for the extraction of potential basis (reference) spectra for LLS fitting. Panel B shows the Si 2p composite spectrum from the entire image area which indicates the presence of multiple chemical states with overlapping spectra. Panel C shows the three basis spectra extracted from the areas defined in Panel A. Panel D shows the chemical state images created using the three basis spectra and LLS fitting to interrogate the spectra at each pixel of the Si 2p image.

Results: The SXI and elemental intensity images displayed in Figure 1 clearly show the locations of multiple regions of interest on the semiconductor device structure. The bond pads are shown to have W, Si, and O at the surface. In addition, regions with the collocation of Si and O, and Si and N are observed. Since Si is collocated with three different elements (W, O, and N) LLS fitting was applied to extract basis spectra from the Si 2p image data set and create chemical state images based on these spectra.

The composite spectra displayed in Figure 2 provide additional interpretation of the surface chemistry. The W 4f binding energies for the peaks found in Panel A of Figure 2 reveal that the tungsten is present at the surface with oxide and metallic chemistries. The N 1s binding energy for the peak in Panel C of Figure 2 is consistent with a silicon oxynitride. The O 1s peak shape and binding energy value for the peak in Panel D of Figure 2 is consistent with a silicon oxynitride and silicon oxide. The composite Si 2p peak shape and binding energy values found in Panel E of Figure 2 indicate multiple silicon chemical states co-exist over the imaged area of this sample.

The SXI and elemental images provided the ability to observe and select regions of the Si 2p image from which to extract 128 channel spectra for chemical interpretation and LLS fitting. The extracted spectra are created by adding the spectra from all the pixels within the selected regions of interest. Panel A of Figure 3 shows the three regions of interest for the extraction of spectra. The spectra obtained from the three regions are displayed in Panel C. These three spectra appear to represent a reasonable set of basis spectra for LLS fitting the spectra contained in the Si 2p image data set. The resulting LLS chemical state fitting of the 65,536 spectra, each with 128 channel spectra, provided three chemical images that are displayed in a color overlay mode in Panel D. The Si chemical state images appear to provide a complete chemical state interpretation of the Si 2p image data, with phases of Si oxynitride, Si oxide, and a region that is a mixture of tungsten silicate and tungsten silicide. The chemical state images also correlate with the O 1s, N 1s and W 4f elemental intensity images shown in Figure 1.

Conclusion: Chemical state imaging based on spectra at each image pixel with 128 data channels were shown to be very useful in identifying multiple regions with different chemistries on the surface of the semiconductor device structure. The high speed with which these images were obtained is a result of the high collection efficiency of the spectrometer combined with the benefits of the focused scanning x-ray source used by *Quantero II* and *VersaProbe II* scanning XPS microprobes. The robust dual beam charge neutralization apparatus that is an integral part of these instruments ensures that chemical state imaging can be applied to both inorganic and organic materials.

