

## **Depth Profiling using XPS**

While XPS is a surface sensitive technique, a depth profile of the sample in terms of XPS quantities can be obtained by combining a sequence of ion gun etch cycles interleaved with XPS measurements from the current surface. An ion gun is used to etch the material for a period of time before being turned off whilst XPS spectra are acquired. Each ion gun etch cycle exposes a new surface and the XPS spectra provide the means of analysing the composition of these surfaces.



Figure 1: Segment of an XPS depth profile.

The set of XPS spectra corresponding to the oxygen 1s peaks from a depth profile experiment depicted logically in Figure 1 are displayed in Figure 2. The objective of these experiments is to plot the trend in the quantification values as a function of etch-time.





The actual depth for each XPS analysis is dependent on the etch-rate of the ion-gun, which in turn depends on the material being etched at any given depth. For example, the data in Figure 2 derives from a multilayer sample consisting of silicon



oxide alternating with titanium oxide layers on top of a silicon substrate. The rate at which the material is removed by the ion gun may vary between the layers containing silicon oxide and those layers containing titanium oxide, with a further possible variation in etch-rate once the silicon substrate is encountered. The depth scale is therefore dependent on characterizing the ion-gun, however each XPS measurement is typical of any other XPS measurement, with the understanding that the charge compensation steady state may change between layers.



Figure 3: XPS Depth Profile of silicon oxide/titanium oxide multilayer sample profiled using a Kratos Amicus XPS instrument.

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Etch	Ti 2p	Si 2p	0 1s	C 1s 🔥
0	Ti 2p/2	Si 2p/3	O 1s/4	C 1s/5
150	Ti 2p/8	Si 2p/9	O 1s/10	C 1s/11
300	Ti 2p/14	Si 2p/15	O 1s/16	C 1s/17
450	Ti 2p/20	Si 2p/21	O 1s/22	C 1s/23
600	Ti 2p/26	Si 2p/27	O 1s/28	C 1s/29
750	Ti 2p/32	Si 2p/33	O 1s/34	C 1s/35
900	Ti 2p/38	Si 2p/39	O 1s/40	C 1s/41
1050	Ti 2p/44	Si 2p/45	O 1s/46	C 1s/47
1200	Ti 2p/50	Si 2p/51	O 1s/52	C 1s/53
1350	Ti 2p/56	Si 2p/57	O 1s/58	C 1s/59
1500	Ti 2p/62	Si 2p/63	O 1s/64	C 1s/65
1650	Ti 2p/68	Si 2p/69	O 1s/70	C 1s/71
1800	Ti 2p/74	Si 2p/75	O 1s/76	C 1s/77
1950	Ti 2p/80	Si 2p/81	O 1s/82	C 1s/83
2100	Ti 2p/86	Si 2p/87	O 1s/88	C 1s/89
2250	Ti 2p/92	Si 2p/93	O 1s/94	C 1s/95
2400	Ti 2p/98	Si 2p/99	O 1s/100	C 1s/101
2550	Ti 2p/104	Si 2p/105	O 1s/106	C 1s/107
2700	Ti 2p/110	Si 2p/111	O 1s/112	C 1s/113
2850	Ti 2p/116	Si 2p/117	O 1s/118	C 1s/119
3000	Ti 2p/122	Si 2p/123	O 1s/124	C 1s/125
3150	Ti 2p/128	Si 2p/129	O 1s/130	C 1s/131
3300	Ti 2p/134	Si 2p/135	O 1s/136	C 1s/137
3450	Ti 2p/140	Si 2p/141	O 1s/142	C 1s/143
3600	Ti 2p/146	Si 2p/147	O 1s/148	C 1s/149
3750	Ti 2p/152	Si 2p/153	O 1s/154	C 1s/155
3900	Ti 2p/158	Si 2p/159	O 1s/160	C 1s/161
4050	Ti 2p/164	Si 2p/165	O 1s/166	C 1s/167 🗸
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Figure 4: Logical structure of the VAMAS blocks in an XPS depth profile.

The XPS depth profile in Figure 3 is computed from the VAMAS file data logically ordered in CasaXPS as shown in



Figure 4. The O 1s spectra displayed in Figure 2 are highlighted in Figure 4. One point to notice about the profile in Figure 3 is that the atomic concentration calculation for the O 1s trace is relatively flat for the silicon oxide and titanium oxide layers, in contrast to the raw data in Figure 2, where the chemically shifted O 1s peaks would appear to be more intense for the silicon oxide layers compared to the titanium oxide layers. This observation is supported by the plot of adjusted peak areas in Figure 5, where again the O 1s trace is far from flat. The profile in Figure 3 is far more physically meaningful than the variations displayed in Figure 5. Normalization of the XPS intensities to the total signal measured on a layer by layer basis is important for understanding the sample. This example is a good illustration of why XPS spectra should be view in the context of the other elements measured from a surface.

The details of how to analyze a depth profile in CasaXPS are discussing at length in The Casa Cookbook and other manual pages available from the Help option on the Help menu.



Figure 5: Peak areas scaled by RSF used to compute the atomic concentration plots in Figure 4.