Application Note #1

High Energy XPS (HAXPES)

Background

Most laboratory x-ray sources have anodes comprised of Al or Mg, primarily giving rise to Al Kα or Mg Kα radiation, yielding photon energies of 1486.6 eV and 1253.6 eV respectively.

Despite higher energy sources being available, their use has been somewhat limited due to their larger inherent linewidth (Table 1), difficulty in monochromatising and a limited knowledge on sensitivity factors, analyser transmission functions and other experimental parameters required for accurate quantification.

Nevertheless, the use of higher energy photons such as those from Ag Lα or Cr kα x-ray sources can greatly aid qualitative analysis.

X-ray Line	Photon Energy (eV)	Line Width (eV)
Mg kα	1253.6	0.7
Al kα	1486.6	0.85
Al kα (monochromatic)	1486.7	0.3
Zr Lα	2042.4	1.7
Ag Lα	2984.3	2.6
Ag Lα (monochromatic)	2984.3	0.6
Ti kα	4510.9	2.0
Cr kα	5417.0	2.1

Table 1. *Photon energies and line widths of some characteristic X-ray lines.*

Common on the current generation of photoelectron spectrometers are dual monochromatic Al/Ag sources, since the same monochromator quartz crystal can be used for 1st (Al) and 2nd (Ag) order Bragg diffraction to obtain monochromatic kα or Lα radiation respectively.

Sampling Depth and Energy Range

The photon energy of Ag Lα (2984.3) eV is approximately twice that of Al Kα (1486.6 eV). This greater photon energy not only allows the excitation of higher binding energy core levels for some elements (Table 2), but also the ability to analyse deeper (buried) layers due to a decrease in electron attenuation length with increasing photoelectron energy [1].

For example, using the TPP2M method for calculating the inelastic mean free path (IMFP), then for a C(1s) peak, with a binding energy of 285 eV, the IMFP using Al Kα X-rays is 3.3 nm at a kinetic energy (KE) of 1201 eV, whilst for Ag Lα this is increased to 6.3 nm (kinetic energy of 2699 eV) [2].

Example – Molybdenum Disulphide (MoS_2)

Figure 1 shows wide scans from an argon cluster-cleaned sample of MoS_2, acquired using both Al and Ag radiation, whilst figure 2 shows high resolution scans for the Mo(3d)/S(2s) region. For clarity the
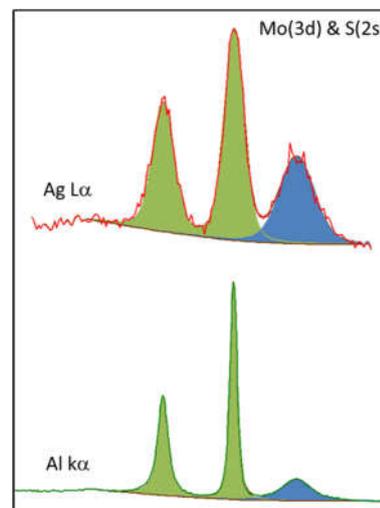
spectral intensity has been normalised, but importantly the excitation of the S(1s) and Mo(2p) core-levels are clear in figure 1, whilst the greater concentration of the S(2s) peak is evident in figure 2.
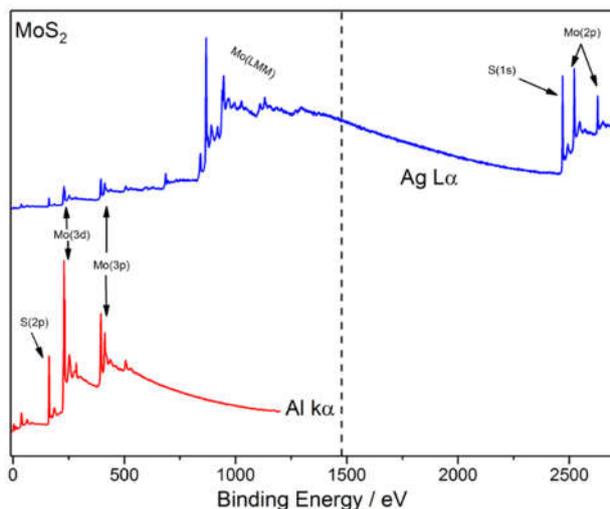
Figure 1. Al Kα (red) and Ag Lα (blue) survey spectra for MoS$_2$

Figure 2. High resolution spectra for Mo(3d) and S(2s)

Deeper Core-Level Analysis

One clear advantage of using a higher energy source is the ability to study other core-levels [3]. The now readily available Ag Lα source, allows access to the core-levels shown in table 2. Comparison of two different peaks from the same element can greatly aid identification of such buried elements.

Core-Line	Elements
1s	Al - Cl
2s	As - Mo
2p	Br - Ru
3s	Pr - Re
3p*	Sm - Tl
3d*	Tm - Rn

Table 2. Core-lines and elements accessible only by using Ag Lα X-rays. [3]

(*at least one half of doublet accessible)

References

[1] M.P. Seah, W.A. Dench, *Surf. Interface Anal.,* 1 (1979) 2

[2] Quases-IMFP-TPP2M (www.quases.com); see also S. Tanuma, C.J. Powell, D.R. Penn, *Surf. Interface Anal.*, 21 (1994) 165

[3] X-Ray Data Booklet LBNL/PUB-490 Rev.2 Jan 2001 (http://xdb.lbl.gov)