Applications Note

Eliminating Core Line/Auger Peak Overlap using Different Photon Energies

Overview

GaN is one of many materials which are difficult to analyze with the conventional Al Kα X-ray source due to a strong overlap between the N 1s core line and the Ga LMM Auger series. This brings difficulties with accurate quantification and also chemical state assignment. In this applications note, GaN was analyzed using different X-ray excitation sources with the aim of shifting the binding energy position of the Ga LMM Auger series to prevent its interference with the N 1s region. Automation of changing between the Al Kα and Ag Lα excitation sources when using the Kratos AXIS Supra+ is an added benefit.

Introduction

The preparation of high quality GaN bulk and thin film single crystal materials is an important prerequisite for the research and development of high performance nitride light-emitting and electronic devices[1]. X-ray Photoelectron Spectroscopy (XPS) is an important surface analysis tool which is widely used to analyse thin film materials to obtain information regarding accurate sample quantification and chemical state assignment of the elements present.

A typical issue with the conventional monochromatic Al Kα X-ray source is that overlap can occur between key elements present in a material. This brings difficulties with accurate quantification and also assigning chemical states as one cannot distinguish between the peaks overlapping within the region of interest. This is true for GaN materials where the Ga LMM Auger series strongly overlaps with the N 1s region, not only affecting the chemical analysis of nitrogen but also providing complications with quantification. Although a differ-

ent photon energy will cause a shift in the binding energy of the Auger series, switching to an achromatic Mg source is sometimes undesirable as a result of X-ray satellites in the spectrum, so other avenues need to be pursued.

In this applications note, GaN is characterized by XPS using 3 different X-ray sources, monochromatic Al Kα, monochromatic Ag Lα and achromatic Mg Kα, to overcome this issue.

Experimental

GaN was analysed using the state-of-the-art, multi-technique Kratos AXIS Supra+ spectrometer, fitted with a monochromatic Ag/Al and achromatic Mg X-ray sources. Survey spectra were acquired over a large energy range, whilst high resolution region spectra were acquired over a small energy range.

Standard X-ray sources for laboratory-based instruments are Al Kα or Mg Kα which provide photons with an energy of

1486.6 eV and 1254.6 eV, respectively. The Ag Lα excitation source has a photon energy of 2984.2 eV, roughly twice that of Al Kα, and therefore the Ag Lα monochromatic source uses second order diffraction of the same quartz crystals. Automation of the X-ray source and monochromator mirror through the ESCApe software allows seamless switching between the Al Kα and Ag Lα excitation sources, being completely computer-controlled with no manual input required.

The greater photon energy of the Ag Lα X-ray source allows excitation of additional, higher binding energy core lines for some elements, as seen in Figure 1. It is also possible to analyze deeper into a material as a result of the decrease in attenuation length with increasing photoelectron energy[2].
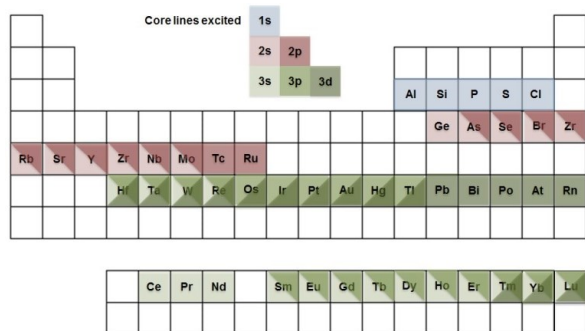

Figure 1. Additional, higher energy core lines accessible with Ag Lα excitation source.

Results and Discussion

A survey spectrum of GaN was recorded using the 3 different excitation sources. As can be seen from the blue spectrum in Figure 2, the Ag Lα excitation source can excite additional core lines up to a binding energy of 2984 eV.
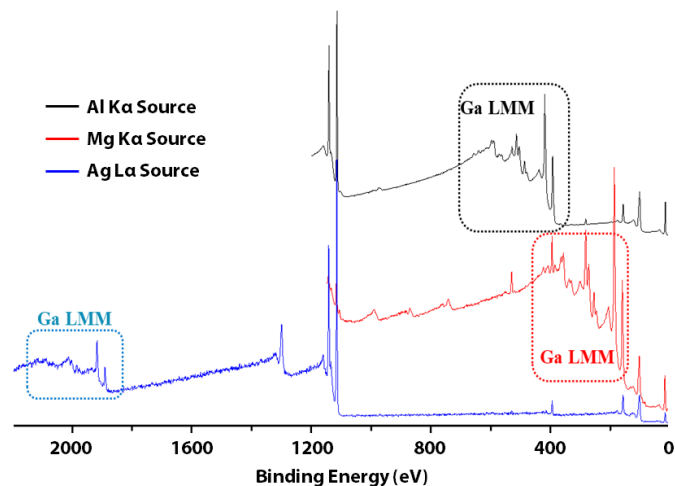

Figure 2. Survey spectra of GaN using monochromatic Al Kα (black)/Ag Lα (blue) and achromatic Mg Kα (red).

As a result of the photoemission process, Auger electron can be emitted following an internal rearrangement of an outer shell electron to fill the core vacancy. In some cases, Auger peaks of one element overlap with the characteristic photoelectron lines

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of other elements, resulting in an interference of data analysis. As the kinetic energy of Auger electrons is irrespective of the photon energy, the selection of a suitable X-ray excitation source can play a key role in the separation of Auger and core-level peaks.
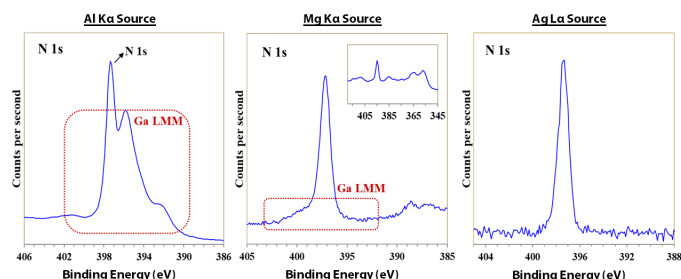

Figure 3. N 1s spectra acquired with a) monochromatic Al Kα, b) achromatic Mg Kα and c) monochromatic Ag Lα X-ray sources.

Figure 3 reveals the N 1s region spectra for each excitation source. As can be seen from Figure 2a and 2b, the Ga LMM Auger series strongly overlaps with the N 1s photoelectron line. This makes it difficult for accurate quantification and chemical state analysis of the nitrogen present in this sample. However, when the Ag Lα excitation source is used, the Ga LMM Auger series shifts to a higher binding energy region, which eliminates its interference with the N 1s peak at the low binding energy region. Chemical state analysis of the N 1s peak can now be obtained, along with accurate quantification using the Cant Relative Sensitivity Factors (RSF)[3], as seen in Table 1.

Element	peak	BE (eV)	RSF	Atomic Conc. %
C	1s	285.0	1.00	**14.25**
O	1s	532.7	2.93	**11.37**
N	1s	397.7	1.81	**36.26**
Ga	$2p_{3/2}$	1117.9	17.89	**38.12**

Table 1. Quantification of GaN using monochromatic Ag Lα excitation source and Cant Relative Sensitivity Factors[3].

Conclusions

When the high energy Ag Lα excitation source is used, the Ga LMM auger series is separated from the N 1s region. This allows the chemical state analysis of nitrogen to be determined as well as accurate sample quantification. This concept can be expanded to other materials which experience similar overlapping regions, with the added benefit of automated switching between the Al Kα and Ag Lα excitation sources on the AXIS Supra+.

Acknowledgements

References

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[2] M. P. Seah *et al.*, Surf. Interface Anal., 1979, **1**, 2.
[3] A. G. Shard *et al.*, Surf. Interface Anal., 2019, **51**, 763-773.