Application Note

Keywords: Thin film, Buried interface characterization, Oxide electronics, Ferroelectric

Revealing subsurface chemistry and defect dynamics with HAXPES

Introduction

Understanding buried interfaces is essential for optimizing electronic, magnetic, and optoelectronic devices, especially as modern materials systems increasingly rely on nanometer-thick functional layers protected by overcoats or encapsulation. However, conventional surface-sensitive techniques like X-ray Photoelectron Spectroscopy (XPS) often fail to access chemical information beneath these protective layers.

Hard X-ray Photoelectron Spectroscopy (HAXPES) addresses this challenge by enabling non-destructive analysis of chemical states and band structure at depths of 10–30 nm and beyond. The Scienta Omicron laboratory HAXPES instrument delivers synchrotron-quality performance in a compact, lab-based system through a high-brightness monochromatic X-ray source and optimized optics. This enables routine, high throughput buried interface studies without the need for synchrotron access.

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Methods

In this application, the chemical and electronic structures of buried interfaces were examined using the Scienta Omicron laboratory HAXPES instrument system operating at 9.25 keV excitation energies.
Two key samples studied:

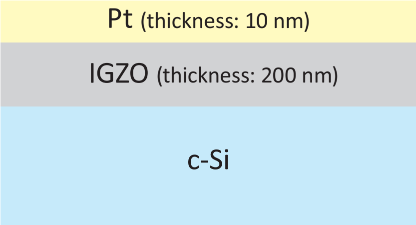

Figure 1: An IGZO thin film capped with a ~10 nm Pt layer (Meiji University).[1]

The IGZO/Pt sample was analyzed to probe valence band states and the oxidation environment beneath the Pt layer, critical for understanding charge transport.

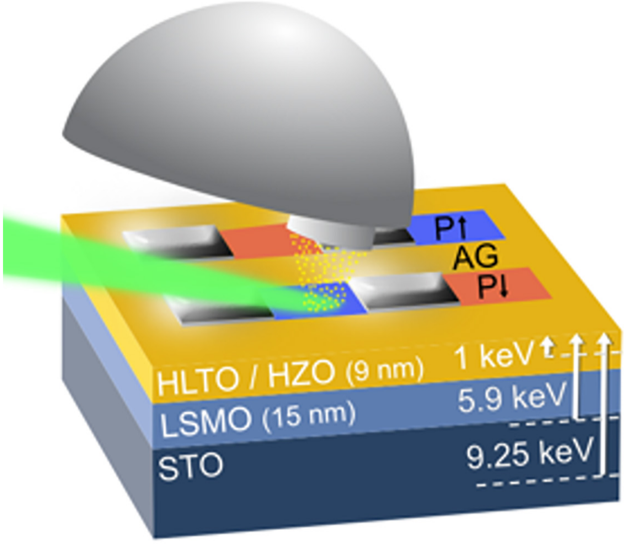

Figure 2: A HfO_2-based ferroelectric film exhibiting oxygen vacancy migration behavior (University of Manchester).[2]

The HfO_2 film was studied using angle-resolved HAXPES to characterize the depth distribution of non-lattice oxygen species (NL-O), which influence ferroelectric behavior and long-term reliability.

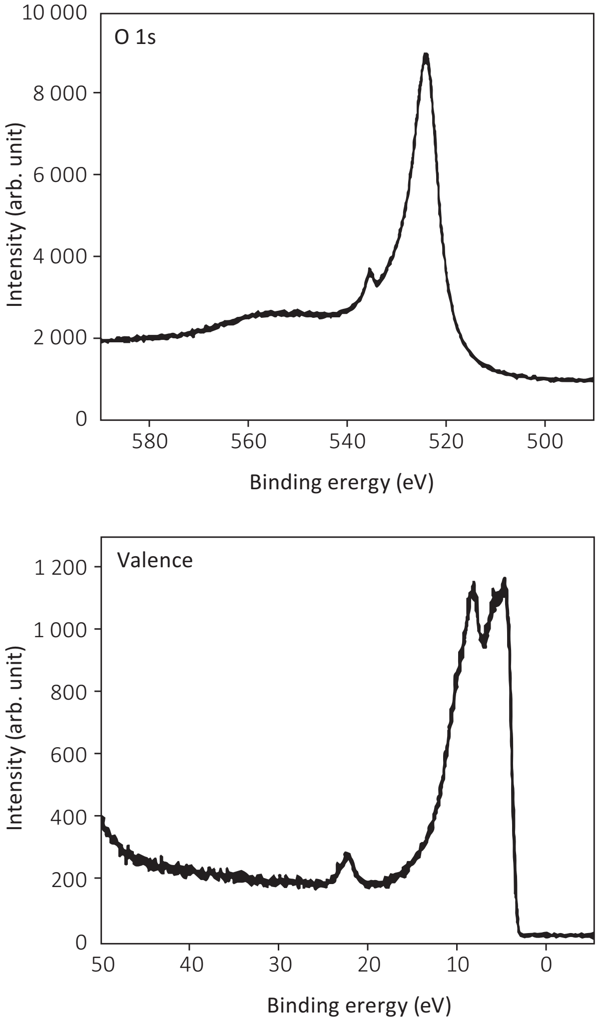

Figure 3: O1s and valence band spectra from below IGZO below a Pt capping layer, recorded with Scienta Omicron laboratory HAXPES instrument.[1]

All data were collected on a Scienta Omicron laboratory HAXPES instrument with a MetalJet Ga excitation source, without the need for synchrotron radiation.

Results and Discussion

For the IGZO/Pt sample, HAXPES spectra collected at 9.25 keV revealed the valence band spectra and oxidation states that are not accessible under the Pt cap with lower photon energies. By varying the material mixing ratio and deposition parameters of the sample, the origin of the electrical characteristics of IGZO can be understood.

In the case of the HfO_2 ferroelectric film, angle-resolved HAXPES enabled a depth profile of the NL-O species. The NL-O peak at approximately binding energy 532 eV in the O-1s spectra reduces with increasing depth (Fig 4a & 4d), indicating that the NL-O is primarily concentrated within the HZO, not the LSMO. Non-destructive, depth-resolved chemical mapping such as this example, is difficult or impossible with traditional XPS techniques.

Furthermore, the Hf-3d and Zr-2p spectra (Fig 4b & 4c) exhibit not only peak shifts but also changes in peak shape reflected by a ≈0.2 eV larger full-width-half-maximum (FWHM) for the P-up conditions. This points to a reduction of Hf/Zr in the P-up state that increases the proportion of lower BE HfOx and ZrOx peaks.

These case studies demonstrate HAXPES's capacity to monitor chemical states, electronic structure, and defect distributions within buried layers, making it an essential tool for advanced interface engineering.

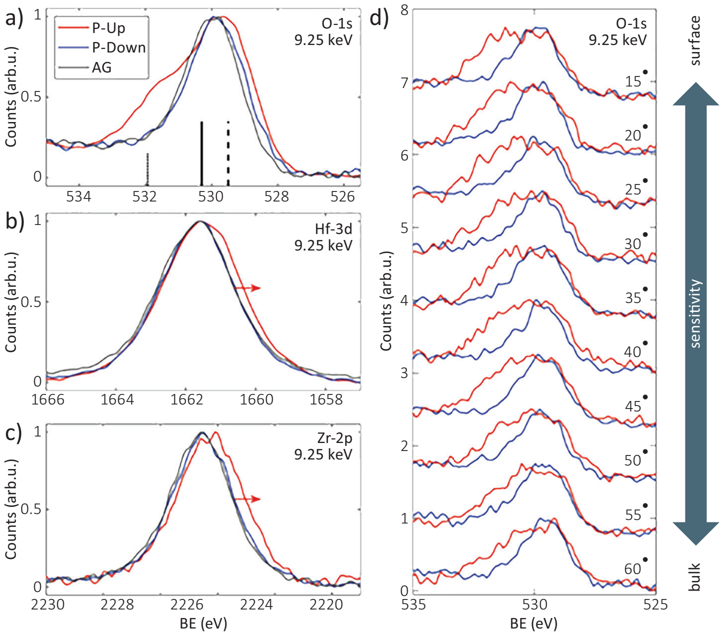

Figure 4: Angle-resolved HAXPES of a HfO_2-based ferroelectric film at 9.25 keV reveals polarization-dependent chemical shifts and a that non-lattice oxygen is primarily concentrated within the HZO layer.[2]

Conclusion

Buried interfaces govern many of the functional properties of modern devices but are challenging to characterize using conventional tools. HAXPES offers a powerful, non-destructive alternative by accessing deeper core levels and revealing buried chemical states with high fidelity.

TheScienta Omicron laboratory HAXPES instrument enables routine, lab-scale exploration of buried interfaces with capabilities previously limited to synchrotron facilities. As device architectures grow more complex, tools like HAXPES will be essential for driving innovation in semiconductors, oxide electronics, memory devices, and energy storage technologies.

References:

1 Internal data, Meiji Univeristy, Japan

2 Hill, M.O., MacManus-Driscoll, J.L., 2024. Advanced Materials 36, 2408572. CC BY 4.0 doi: 10.1002/adma.202408572.)

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