Applied Surface Science
Room 319 - Session AS-TuM

Applied Surface Science in Action I

Moderators: Dr. Michael Eller, University of Mississippi, **Dr. Samantha Rosenberg**, Kairos Power

11:00am **AS-TuM-13 Considerations when Developing Standards and Tools for Surface Chemical Analysis***, **Justin Gorham**, Donald Windover,* National Institute of Standards and Technology (NIST) **INVITED**

Surface chemical analysis, like other disciplines, rely on harmonized methods and benchmarking materials in order for results from the same technique to be reproducible from institute to institute. These harmonized methods are often incorporated into documentary standards which contain the details analysts require to conduct a process (e.g. prepare sample(s); calibrate the tool(s); conduct the measurement(s); analyze data; reporting requirements; etc.). Benchmarking materials are often co-developed during standards work as either a classification of reference materials or simply materials of known purity. As the name implies, these benchmarking materials are often employed as a tool for checking/calibrating a given property of a tool (e.g. linearity of energy scale). This presentation will focus on considerations and tools employed in the development of standards from a surface analysis perspective. Discussion will be held on both the development and maintenance of standards. Additionally, discussion will focus on the use case of NIST benchmarking materials known as research grade test materials (e.g. Hafnium oxide, Titanium Nitride, etc), currently under development, to advance measurements in the semiconductor community specifically as it pertains X-ray based measurements (e.g. XRR, XPS, XRF).

11:30am **AS-TuM-15 Might a Tiered Approach to Reviewing and Reporting Help Improve the Quality of XPS Results Appearing in Publications?***, **Don Baer,*** Pacific Northwest National Laboratory

Anecdotal evidence, confirmed by detailed analysis, highlights widespread inadequacies in XPS data and analysis reported in scientific literature. As XPS is increasingly utilized across various fields, researchers without specialized XPS knowledge often collect, analyze, and report data. These papers are often reviewed by experts in the subject matter, not in XPS, leading to missing or incomplete instrumental, data, and analysis information appearing in journals. Consequently, the quality and reliability of XPS results are difficult to assess, and flawed data is frequently published. Although this issue is not unique to XPS, this talk focuses on the reviewing and reporting of XPS information.

Surface analysis experts have worked to provide guidelines for less experienced XPS users. However, there remains a gap between the information reported in journals, what would comply with ISO and ASTM standards, the expectations of reviewers, and what is really needed. Research by Karel Gaskel revealed that most standard-required information is not reported, reflecting a disconnect between ideal reporting practices and practical journal requirements. Standards often focus on full repeatability, which can be burdensome and not always relevant, yet more information is needed than is typically provided to ensure data quality and relevance.

To address these challenges, a tiered approach to reviewing and reporting XPS data is suggested for discussion. A model might include three levels: i) **Credibility Level:** Data follows generally accepted practices and is adequate for its stated purpose in journals or reports, especially when XPS is not a primary analysis method used in the paper; ii) **Archive Level:** Data and analysis are of high quality, with sufficient detail about the instrument, sample, and analysis to allow for inclusion in databases and to provide context and purpose; **Reference/Fully Repeatable Level:** Full information is provided, enabling experts to replicate experiments and qualify the data as "reference data" of standard quality.

The need for thorough and appropriate reporting grows as artificial intelligence and data archiving become more prevalent. Adequate information is necessary for AI systems to identify high-quality data, and for archives to maintain meaningful records. A tiered approach might offer a practical guide for improving both the reporting and review of XPS data, aligning reporting requirements with the intended use and ensuring data quality across various applications. The challenge is identifying what each of these, or other, levels would mean in practice and how they might be described with clarity.

11:45am **AS-TuM-16 Strategies for Reducing Charging of Insulating Samples in Auger Electron Spectroscopy***, **Juergen Scherer,*** Physical Electronics

Auger Electron Spectroscopy (AES) is a powerful surface-sensitive analytical technique widely used to probe the elemental and chemical composition of materials at the nanoscale. Its high spatial resolution makes AES uniquely valuable for applications ranging from microelectronics and thin films to failure analysis and advanced materials. However, a persistent challenge in AES is the analysis of materials that are insulating or contain insulating regions, which represent a large and growing fraction of technologically relevant materials. Charge accumulation under electron beam irradiation can lead to spectral distortion, peak shifting, signal loss, and, in severe cases, the inability to obtain meaningful data.

This presentation discusses practical strategies for reducing and managing charging effects during AES analysis of insulating and heterogeneous samples. Emphasis is placed on understanding the physical origins of charging phenomena and how instrument configuration, experimental conditions, and sample preparation choices can be leveraged to mitigate their impact. Through illustrative examples, the talk highlights how thoughtful control of measurement parameters can substantially improve data quality, reproducibility, and reliability when working with challenging samples. By focusing on realistic scenarios encountered in routine AES measurements, this work aims to provide users with actionable insights for extending the applicability of AES to a broader class of insulating and heterogeneous materials.

12:00pm **AS-TuM-17 The Binary Residual Map and the Automated Determination of the Transfer Function Cutoff for the Fourier Filtering of X-ray Photoelectron Spectroscopy Data***, **Matthew Linford**, Alvaro Lizarbe, Maksym Gerashchenko, Tyler Andersen, Jonathan Nelson,* Brigham Young University*; David Aspnes,* NC State

We recently proposed that the Fourier denoising of X-ray photoelectron spectroscopy (XPS) data may have a legitimate place in XPS data processing (*J. Vac. Sci. Technol. A,* **2025**, *43*, 033401). For example, the denoising of spectra becomes critical when they are to be used for training artificial intelligence (AI) systems. In this talk, we discuss two new data analytical tools we have developed that greatly facilitate the Fourier denoising of XPS and other types of data. The first is the Binary Residual Map™. The binary residual map color codes the residuals from large numbers of fits or smooths and combines them into a single figure. The transition in a binary residual map where longer runs of a single color disappear is generally where good fitting or denoising is taking place. In addition, we have developed an algorithm, which we will discuss, that finds a reasonable position for the transfer/filter function in reciprocal space for denoising. This feature will be important both for newer users that may be unsure about Fourier analysis and also for fully automating the denoising of XPS data.

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