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Applied Surface Science Division
Room On Demand - Session AS-Invited On Demand

Applied Surface Science Invited On Demand Session

AS-Invited On Demand-1 Hard Targets: Developing Tools for Quantitative HAXPES, ***David Cant,*** National Physical Laboratory, U.K. **INVITED**

'Soft' x-ray based XPS, using aluminium or magnesium anodes, has been a workhorse of surface analysis labs for decades. Over this time, substantial efforts have been placed in the development of tools such as sensitivity factors, transmission calibration procedures, parameter databases, simulation software, interpretation formulae, and more. Thanks to such tools, the results obtained from 'soft' XPS, with careful analysis, can provide a strong, quantitative understanding of samples in terms of the relative concentration of elements and their chemistry within, typically, the top ~10 nm of material. Nevertheless, sometimes 10 nm is not enough.

Until recently, photoelectron spectroscopy of materials beyond this topmost region of the surface would require either destructive depth profiling of the sample or the use of synchrotron light sources; the former carries its own metrological trials and tribulations, as well as ruining a perfectly good sample, while the latter introduces a plethora of complexities which render calibration difficult, and careful experimental design and reference materials a necessity. However, recent developments in the design of instruments utilising higher-energy, or 'hard' x-ray anodes have begun to make synchrotron-energy XPS instruments more readily available in the lab. This will allow more analysis of samples that previously might have been restricted to synchrotron studies; for example in non-destructive depth-profiling of coated samples such as core-shell nanoparticles, particularly those with shells beyond the ~10 nm limit of 'soft' XPS. Yet with new instruments come new issues; transmission function calibrations that work for the 0 - 1400 eV energy range are not much use for a spectrum that stretches some KeV beyond, and relative sensitivity factors for each new photon energy are needed, particularly given the cornucopia of new core levels made available and the increased breadth of sensitivity at higher photon energies.

Here we discuss developments towards more trustworthy, quantifiable XPS and HAXPES measurements.The development of theoretical sensitivity factors for silver and gallium x-ray sources is described, as well as demonstrating their validity in depth-profiling of samples well beyond the depth achieved by aluminium. We discuss developments in straightforward transmission-function calibrations of standard aluminium sources by the use of a mathematically-defined reference spectrum, as well as progress towards transmission calibration of higher energy sources for which reference spectra do not yet exist. From these developments, the possibility of a 'universal' calibration and sensitivity scheme for HAXPES systems at a range of energies is proposed.

AS-Invited On Demand-19 ASSD 2020 Peter M.A. Sherwood Mid-Career Professional Award Talk: Innovations in Biological, Nanoscale, and Nuclear Materials Analysis with SIMS, ***Christopher Szakal,*** National Institue of Standards and Technology **INVITED**

This presentation will highlight advances in secondary ion mass spectrometry (SIMS) to address measurement gaps in the characterization of biological, nanoscale, and nuclear materials as related to the 2020 Peter M.A. Sherwood Mid-career Professional Award. Presented work will focus on the development of methods needed to answer questions related to single cells, nanomaterial surface chemistry, and micrometer-sized actinide particles. Despite the wide range of applications, these are distinct examples of how time-of-flight (TOF)-SIMS and large geometry (LG) magnetic sector SIMS can add value to multiple scientific fields.

AS-Invited On Demand-25 The Role of Photoelectron Diffraction Effects on the Flat Surface State Bands Close to the Fermi Level: Revisiting the Si(111) 7x7 Surfaces, ***María C. Asensio,*** Materials Science Institute of Madrid (ICMM), Spanish Scientific Research Council (CSIC), Spain **INVITED**

Lately, seminar discoveries of new surface states of matter have been reported almost every year, disclosing new materials such as topological insulators and superconductors, high-temperature superconductivity in hydrates under pressure and pnictides, and a large diversity of many-body phases in the flat bands of Moire lattices of a few atomic layers of two-dimensional materials. The continuing search for higher degrees of miniaturisation and the rise of new quantum layer materials such as silicene, graphene, and topological matter, drives an accruing need to understand the electronic structure of systems dominated by surface states confined just in a few atomic layers. The unconventional evolution of the electronic properties of reducing material to a few-layer plays a central role in microelectronic devices silicon technology. Moreover, unravelling the peculiar attributes of the electronic properties of the upper layers of silicon with their characteristic two surface state bands may have a remarkable impact on the transport properties of silicon-based nano-devices that are crucial for future high-speed electronics nanotechnologies.

In this presentation, the role of localisation of typical surface state bands of the 7x7 reconstructed surfaces of silicon will be revised. In particular, the metallic character of the surface bands close to the Fermi level will be investigated, taking into account the influence of photo-diffraction effects on the Fermi surface topology measured using Angle-resolved photoemission spectroscopy (ARPES). In contrast to previous studies, our findings show that the two-dimensional intensity patterns at constant energy close to the Fermi level are due to strong photo-diffraction effects modulated by the photoemission matrix element, instead due to the Fermi level crossing of the metallic delocalised surface states bands of the outmost surface state of the (7x7) reconstruction. Combining ARPES experiments and multiple scattering calculations, our results unravel a comprehensive understanding of the orbital character of the adatoms and rest-atoms in terms of a remarkable atomic localization of the Si (111) 7x7 reconstructed surface state bands lying at the silicon bulk gap.

AS-Invited On Demand-37 Hardware and Data Analysis Methods for Integrating TEM and Atom Probe Tomography, ***Brian Gorman,*** *E. Supple, G. Burton,* Colorado School of Mines **INVITED**

Errors during APT data reconstruction are still limiting widespread acceptance of APT as a quantitative imaging technique. There are many factors contributing to these reconstruction inaccuracies, but they include empirical estimation of specimen geometry based upon the assumed evaporation field, inaccurate assumptions of the ion trajectories, and magnification changes due to varying field evaporation characteristics at heterointerfaces. Utilizing ex-situ correlative TEM imaging with APT has been shown to improve the accuracy of data reconstruction through the quantification of many of the reconstruction variables, including radius, shank angle, atomic spacing, detection efficiency, image compression factor, and field of view. However, the full use of TEM has not yet been applied to the APT experiment as a wealth of other information are useful and readily attainable. In order to further improve APT as a quantitative imaging and analysis technique, hardware enabling in-situ APT within a TEM objective lens is needed. Our hardware solution enables APT within a TEM objective lens using a modest investment of capital hardware. UHV is obtained using a combination of turbomolecular pumping and a cryogenic trap within the TEM pole gap. Cryogenic specimen temperatures are achieved using a recirculating cryocooler with vacuum transfer to both the side entry stage and the objective lens cryo trap. A commercially available large field of view delay line ion detector assembly fit to a UHV flange is engineered to bolt on the TEM column opposite the specimen holder. Laser integration with commercial in-situ TEM hardware are currently available and being utilized for this instrument. 4-D STEM datasets are utilized in a correlative manner for quantification of the specimen function before the field evaporation experiment. The specimen function contains the real space volume and atom positions (determined from reciprocal space) and can subsequently be created and sliced perpendicular to the evaporation axis. Comparing the specimen function with ion field evaporation maps from the correlative APT experiment in Fourier space allow for quantification of aberrations during the field evaporation experiment. As such, APT may one day become a simple addition to existing electron microscopy hardware.

AS-Invited On Demand-43 High Resolution Angle-Resolved Photoemission Spectroscopy Studies of Quantum Materials, ***Inna Vishik,*** University of California at Davis **INVITED**

Quantum materials are unified by the theme of emergence, whereby the properties of a many-electron system differ from a single-particle description.They often exhibit surprising electronic behavior that is readily revealed by angle-resolved photoemission spectroscopy (ARPES).In this talk, I will discuss recent results on superconducting and topological quantum materials which exemplify how novel materials platforms conspire with this powerful experimental technology to elucidate both new and long-standing problems in this field.

AS-Invited On Demand-55 Synergies between Synchrotron and Lab-Based X-Ray Techniques for the Studies of Complex Materials and Interfaces, ***Alexander Gray,*** Temple University **INVITED**

The several recent studies discussed in this talk were motivated by the challenge of creating new strategies for rational design and control of electronic and magnetic phases of matter at interfaces. The key requirement for the realization of such groundbreaking technology is a clear understanding of how these electronic and magnetic phases arise and evolve at the nanoscale. Gaining such an understanding is not just important for basic science but could be potentially transformative to modern computing. The depth-sensitive synchrotron and lab-based x-ray photoemission techniques developed in the Fadley Group helped elucidate such important phenomena as metal-insulator transitions [1], two-dimensional electron gas [2], and interfacial magnetism [3]. Here, I will discuss several recent studies stemming from this seminal body of work and taking full advantage of multiple complementary x-ray spectroscopic and scattering techniques to probe emergent electronic phenomena at oxide interfaces [3-6].

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