IVS Workshop 2019

"Characterization techniques and exploitation of data in surface and thin film analysis"

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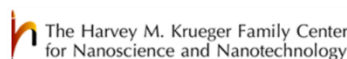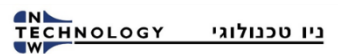
Book of Abstracts

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A New Materials Toolkit: Acquiring and Processing Data Using Multi-Technique Approaches

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Abstract

In recent years there have been large advances in analytical techniques and the use of multi-technique approaches. Consequently we now live in a world in which it is easy to collect large amounts of experimental and computational data in which the data spans physical, chemical and biological sciences. The complexity of samples has also greatly increased, with routine application to tissues, advanced materials, nanosystems, and complex thin films. These samples themselves may be highly heterogeneous and their properties can vary significantly from sample to sample. As a result, the use of the simple data processing routines may not provide good insights into the data obtained.

It is therefore becoming critical to correctly frame the analytical questions that need to be answered. What does the analyst want to know? At what lateral and depth resolution? There are multiple variables such as concentration, topography and chemical composition (elemental or molecular). It is also important to understand the capabilities and limitations of each analytical technique. Such understanding allows the analyst to correctly track the uncertainties from the raw experimental data through to final results. Examples of such uncertainties include the intensities (peak area) in mass spectrometry, and the peak line shapes and areas in x-ray photoelectron spectroscopy (XPS) or infrared spectroscopy. These experimental uncertainties are often not reported because they are difficult to quantify.

To gain further insights multivariate analysis (MVA) methods are often employed after the data is initially processed. Such techniques include principal components analysis (PCA) and multivariate curve resolution (MCR). It is important to note these methods are mathematical transformations, and in theory the original data can be obtained by reversing the transformation. For example, in PCA the loadings of the principal components can be employed to reconstruct the data IF every principal component is known, i.e. 100% of the variance in the dataset is captured. However, MVA data is often employed in a qualitative way, for example by examining images of principal components and identifying the "areas of interest" of a sample. Such components may explain only a few percent of the data which may lead to errors in interpretation. More recently analysis methods such as maximum *a posteriori* (MAP) reconstruction, which include physically motivated models, have been developed to make clearer the connection between the data obtained and the analysis. For example, such MAP analyses allow the deconvolution of matrix effects in secondary ion mass spectrometry (SIMS) from the "pure substance" mass spectrum.

In this talk we shall illustrate and discuss these issues using example SIMS, XPS, and microscopy data from a range of samples including tissues, thin film, heritage materials and nanomaterials.

Electron Spectroscopies as Characterization Tools of Surfaces and Thin Film Heterostructures

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Abstract

Electron spectroscopy proposes unique features as compared to alternative spectroscopies and to the optical analogues in particular. These features originate in both fundamental and practical aspects of the work with electrons and, by exploiting those, a huge range of materials' properties can be probed. Therefore, great potential is predicted for this family of techniques in material research and in the characterization of surfaces in particular. Despite limitations of concern, the use of electron spectroscopy in various research laboratories, academic and industrial, all over the world, is growing exponentially and, in parallel, developmental efforts are taken to address the limitations; so far, with a remarkable success.

In this talk I will describe representative electron spectroscopy techniques and discuss their capabilities in reference to those of analogous optical methods. Specific studies will be shown to exemplify the advantages, the drawbacks and the complementary aspects dealt with when using electrons for spectroscopy. Future directions will be pointed out with respect to recent instrumental and methodological developments.

Ilan Goldfarb, TAU - Analysis of linear defects at single-crystal surfaces by elastic and diffuse scattering in electron diffraction

Diffuse arched streaks often appear in RHEED patterns obtained from various surfaces. These streaks are very different from the straight streaks, perpendicular to the shadow edge, that originate due to a finite size of coherently scattering domains. As elastic scattering is the one most widely used for interpretation of the diffraction data, such diffuse intensity distribution in the reciprocal space is usually ignored.

In this talk I will explain what information is contained in these diffuse intensity streaks, and how it can be used to study linear surface defects. In particular, I will demonstrate RHEED and LEED analysis of two differently reconstructed surfaces of lanthanide (Er and Gd) silicides on Si(111), that nevertheless exhibit similar type of 1D disorder in the form of translational registry shifts between adjacent atomic chains and domains. Such defects in real space cause diffuse intensity planes to appear in the reciprocal space, whose lines of intersection with the Ewald sphere produce the above arched streaks in RHEED patterns. The arc curvature is controlled by the angle between the RHEED electron beam azimuth and the 1D surface features.

Transient phenomena in photocatalysis, as studied by ultrafast FTIR measurements

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Developing of new, highly efficient, photocatalytic materials depends to large extent on better understanding of the physical and chemical phenomena occurring right after photon absorption. Over the years two major techniques have been utilized, using pulsed lasers beams for excitation: time Resolved Microwave Conductivity (TRMC) and UV-Vis absorption and fluorescence spectroscopy.

Here we present a third method for studying the excitation of photoactive and, in particular, photocatalytic materials. The method is based on measuring time resolved changes (2.5 nanoseconds in resolution) in the IR spectra photocatalytic materials following excitation by a pulsed 355 nm laser beam.

In the presentation, the fundamental pros and cons of the method will be described. Results for several photocatalysts ($g-C_3N_4$, $BiVO_4$, ZnS, $BiOCl$) will be presented, revealing spectral transient changes that are sensitive to the phase of the photocatalyst and to its preparation procedure. Results will be compared with theory and will be correlated with photocatalytic measurements and with measurements made by other techniques.

Imaging and Spectroscopy at 10nm Spatial Resolution using s-SNOM

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Scattering-type Scanning Near-field Optical Microscopy (s-SNOM) is a scanning probe approach to optical microscopy and spectroscopy bypassing the ubiquitous diffraction limit of light to achieve a spatial resolution below 10 nanometer. s-SNOM employs the strong confinement of light at the apex of a sharp metallic AFM tip to create a nanoscale optical hot-spot. Analyzing the scattered light from the tip enables the extraction of the optical properties (absorption, reflectivity) of the sample directly below the tip and yields nanoscale images simultaneous to topography. In addition to near-field microscopy the technology has been advanced to enable hyperspectral, nanoscale Fourier-transform spectroscopy (nano-FTIR) using broadband radiation from the far-infrared to the visible spectral range.

Identification of individual contaminants has been demonstrated. Other applications show characterization of embedded structural phases in biominerals or organic semiconductors. The patented modular system design allows for tailored system configurations where the ultimate spectral coverage is achieved by using synchrotron-based broadband IR light sources.

Equipping s-SNOM systems with cw light sources near-field imaging can be performed at time scales of 30-300s per image. Use of material-selective frequencies in the mid-IR spectral range can be exploited to fully characterize polymer blends or phase change polymers with nanometer-scale domains. Quantification of free-carrier concentration and carrier mobility in doped semiconductor nanowires, analysis of 2D (graphene) nanostructures, or study phase propagation mechanisms in energy storage materials is achieved by amplitude- and phase-resolved infrared near-field imaging.