

Undergraduate Poster Session

Room Central Exhibit Hall - Session UN-ThP

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UN-ThP-1 Using Fourier Smoothing to Calculate D-Parameter for Carbonaceous Samples, *Kristopher Wright, M. Linford*, Brigham Young University

Carbon samples reveal much about their properties through surface analysis. X-ray photoelectron spectroscopy (XPS) has proven itself a reliable approach to analyzing surfaces of all material, including carbon samples. We can use the carbon Auger peak as an important tool for characterizing the ratio of sp² to sp³ hybridization of carbon samples. This is accomplished through determining the D-parameter, which is related to the energy difference between the first derivative minima & maxima, and which is directly proportional to the sp²:sp³ ratio of the sample. The D-parameter has many important uses, such as determining graphite versus diamond composition in a material. In the past, the characteristically noisy auger peak has made the D-parameter difficult to determine. In this poster, will be looking at various carbon samples ranging from sp³ carbon (such as diamond), polymers, and sp² carbon samples (like HOPG) using a new approach to determining the derivative of the Auger peak via a Gauss-Hermite Filter. The Gauss-Hermite Filter convolves the data with a transfer function by utilizing Fourier analysis to break down XPS data into its components, then multiplying these by the reciprocal of the transfer function. The result is a minimalization of high frequency noise while preserving the lower frequency components that are characteristic of the signal.

UN-ThP-2 Calcium Lanthanum Sulfide - An Investigation Via X-Ray Photoelectron Spectroscopy, *B. Butkus, Taylor Cook, A. Kostogiannes, A. Cooper, A. Howe, R. Gaume, K. Richardson, P. Banerjee*, University of Central Florida

Calcium lanthanum sulfides (CLS) are crucial in applications requiring high optical transmissivity in the long-wave IR regime. These ternary sulfides, forming solid solutions of CaS and La₂S₃ in a cubic Th₃P₄ phase, exhibit varying cationic vacancies depending on the Ca:La ratio to maintain stoichiometric balance and charge neutrality.

Using X-ray photoelectron spectroscopy (XPS), we analyzed the chemical and bonding states of hot pressed CLS ceramics. Our findings confirm the stoichiometry aligns with the expected Ca:La ~ 10:90 composition, revealing an intrinsic ≥10 at% oxygen impurity even under inert conditions. This suggests oxygen substitution for sulfur, particularly bonding with La, which may influence the material's optical properties as experimentally seen in the lower IR transmission of CLS and development of absorption bands in the long-wave IR regime. The interpretation and conclusions are made from data of over 30 CLS samples with varying compositions. A multivariate analysis of the composition also support the hypothesis that oxygen substitutes for sulfur in the CLS lattice.

This study highlights the persistent challenge of oxygen incorporation in CLS and suggests potential processing modifications to enhance material purity and performance.

UN-ThP-3 Avoiding Common Errors in X-ray Photoelectron Spectroscopy Data Collection and Analysis, *Braxton Kulbacki, J. Pinder*, Brigham Young University; *G. Major*, Texas Instruments; *M. Linford*, Brigham Young University

X-ray photoelectron spectroscopy (XPS) is the most popular surface characterization technique because of its ability to determine the composition and chemical state of the first 5-10 nm of various materials. Although widely used, correct collection procedure, technique and reporting are not widely understood. Experts in other scientific fields use XPS, but are often not experts in XPS as well, so technical errors such as incorrect data interpretation and presentation, incorrect reporting of instrumental parameters, unjustified conclusions and unjustified peak fittings are common. Publications with these errors have made experimental reproduction difficult and have caused a reproducibility crisis. The following presentation is intended to bring awareness to common errors observed. Some common examples include: data collection, peak fitting errors, background errors, data presentation errors and data reporting errors.

UN-ThP-4 Deposition of Cobalt-Doped Zinc Oxide Nanocrystals via Successive Ionic Layer Adsorption and Reaction, *Luis Tomar, K. Ye, S. Xie*, University of Central Florida; *M. Chang, J. Baillie*, University of Washington; *T. Currie, F. Liu, T. Jurca*, University of Central Florida; *D. Gamelin*, University of Washington; *P. Banerjee*, University of Central Florida

Transition metal doped semiconductors are highly desired due to new functionalities enabled by the dopants. For example, Co-doped ZnO has been shown to be a magnetic quantum dot [1]. These materials are typically synthesized in the form of nanoparticles [1], and the ability to synthesize these materials as high-quality thin film is desirable for their applications in optics and electronics. Successive ionic layer adsorption and reaction (SILAR) provides a simple approach to create transition metal doped semiconductors, while providing control over the film thickness and dopant concentration. SILAR works via a series of liquid-phase ionic reactions that are self-limiting, similar to atomic layer deposition [2].

This work aims to synthesize Co-doped ZnO films using a SILAR process. The approach involves adapting the mechanism of solution-based nanoparticle process into a SILAR process. While the solution process involves the rigorous mixing of the precursors to precipitate Co-ZnO nanoparticles, the SILAR process discretizes the use of these compounds into separate dip-coating steps. Thus, by simply controlling the solution concentration and number of cycles, films of various thickness are formed. The films are evaluated using ultraviolet-visible spectroscopy (UV-Vis), scanning electron microscopy, energy dispersive x-ray spectroscopy, and x-ray photoelectron spectroscopy to confirm the successful doping of the isovalent Co²⁺ in the ZnO lattice.

References:

[1] D. A. Schwartz, N. S. Norberg, Q. P. Nguyen, J. M. Parker, and D. R. Gamelin, "Magnetic Quantum Dots: Synthesis, Spectroscopy, and Magnetism of Co²⁺- and Ni²⁺-Doped ZnO Nanocrystals," *Journal of the American Chemical Society*, vol. 125, no. 43, pp. 13205–13218, Oct. 2003, doi: <https://doi.org/10.1021/ja036811v>.

[2] Samantha Prabath Ratnayake, J. Ren, E. Colusso, M. Guglielmi, A. Martucci, and Enrico Della Gaspera, "SILAR Deposition of Metal Oxide Nanostructured Films," *Small*, vol. 17, no. 49, Jul. 2021, doi: <https://doi.org/10.1002/sml.202101666>.

UN-ThP-5 Assessing and Recommending Standards to Improve Reproducibility in Thin Film Analysis; a Multi-Faceted Approach, *Jacob Crossman, M. Linford, J. Pinder*, Brigham Young University

Reproducibility is a key component of the scientific method requiring data collection to be repeatable by oneself and/or others. Also known as replication, reproducibility (or rather, a lack thereof) has established itself as a growing crisis in the scientific community—many studies are being published without providing sufficient information for an outside source to replicate and corroborate findings, thereby reducing confidence in those studies. The variety of scientific fields requiring vacuum technology, including thin film research, are not immune to the reproducibility crisis. Because thin film sciences are crucial to advancements in solar array, computer microchip, and LED technologies, it stands to reason that the scientific community should expect a high degree of transparency and reproducibility from this research. Techniques such as thin film synthesis using ALD or CVD and analysis via methods such as XPS, LEIS, or SE, must be reproducible both internally and externally. This means a researcher should be able to internally reproduce a material or measurement multiple times consistently. Additionally, should that researcher choose to publish his or her findings, he or she should provide sufficient information for an external researcher to reproduce those findings consistently and accurately. This system of reproducibility helps ensure the integrity of research. In this presentation, we pose recommendations and reminders to make sure reproducibility remains central to the research process. To ensure internal reproducibility, we recommend a thorough recording of procedures and tests for consistency. Creatively deploying physical and procedural measures, such as fitment jigs and SOPs are paramount to ensuring internal reproducibility. Externally, we suggest clarity in instrument parameter reporting (such as the tables found in certain SSS articles) and clear, complete supporting information. Any paper published should contain all the information necessary for someone else to perform the same experiment. With recommendations such as these in mind, researchers will continue to prioritize reproducibility and increase the transparency of their research to combat the replication crisis.

Thursday Evening, November 7, 2024

UN-ThP-6 Enhancing the Selectivity of Acetaldehyde Formation Using a Copper-based Model Catalyst, *Joseph Loiselet, A. Baber*, James Madison University

Acetaldehyde is a common intermediate in many industrial chemical syntheses. Current methods of acetaldehyde formation are inefficient and wasteful, leading to low product yields and unwanted by-products. In order to improve acetaldehyde yield and minimize other products, the dry dehydrogenation and dehydration of ethanol was observed using temperature programmed desorption (TPD). These reactions occurred on flat, roughened, and oxidized Cu(111) surfaces under ultrahigh vacuum (UHV) conditions. The reaction of ethanol over each surface was studied, and the oxidized Cu(111) most readily formed acetaldehyde and hydrogen at 350 K. A second reaction pathway formed ethylene and water at 350 K. The selectivity for acetaldehyde production was maintained over 80% throughout consecutive TPDs, yet the yield decreased continuously as the surface became less oxidized. Future experiments will study the reactivity of a partially oxidized Cu(111) sample using UHV-TPD.

UN-ThP-7 Optimizing XPS Analysis with Maximum Entropy for Determination of the D Parameter, *Garrett Lewis*, Brigham Young University

In spectroscopy, the aim is to gather insights through the examination of spectra that are ideally clear of distortions and free from noise. The Maximum Entropy filter is another technique to de-noise XPS that works by preserving both high and low-order coefficients. It achieves this by utilizing the trends established by the low-order Fourier coefficients and projecting them into the white noise region (high-order coefficients). X-Ray Photoelectron Spectroscopy (XPS) is a surface analytical technique used to survey the top 5-10 nm of a sample. In sample analysis, XPS unveils the carbon Auger peak, a product of secondary electron emission upon ejection of a core-level electron from a carbon atom, subsequently filled by an electron from a higher energy level. The carbon Auger peak is pivotal in assessing the D-parameter, a ratio between sp^2 and sp^3 hybridization in carbonaceous materials such as diamond and highly oriented pyrolytic graphite (HOPG). By utilizing the maximum entropy filter, we can demonstrate its effectiveness in enhancing data quality through smoothing, thereby aiding in the determination of the D-parameter via the carbon Auger peak. This improved understanding of material characteristics enhances their potential applications.

UN-ThP-8 Copper by X-Ray Photoelectron Spectroscopy (XPS) at Pass Energies from 10 – 200 eV, *Annika Dean, S. Jafari, M. Linford*, Brigham Young University

X-ray photoelectron spectroscopy (XPS) is an important analytical technique that provides chemical information about surfaces. XPS analyses of metallic copper were performed at different pass energies, ranging from 10 to 200 eV. The pass energy determines the kinetic energy at which the emitted photoelectrons pass through an analyzer and enter the detector. The pass energy determines the energy resolution of the experiment. While survey scans are generally taken at high pass energies, narrow scans are taken at lower pass energies to achieve a higher resolution. Higher resolution can aid in distinguishing between peaks that are close together, such as spin-orbit split peaks, or for identifying fine features in spectra. As expected, lower pass energies result in better resolution but lead to increased noise in spectra. Selecting an appropriate pass energy therefore includes considerations for both the spectral resolution and the desired signal-to-noise ratio.

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