Applied Surface Science
Room: Cochiti A - Session AS2-ThM

Forensics, Failure Analysis, and Practical Surface Analysis
Moderator: I.S. Gilmore, National Physical Laboratory, UK

10:40am **AS2-ThM9 Characterization of Composition C4 Explosives using Time-of-Flight Secondary Ion Mass Sepctrometry (ToF-SIMS) and X-Ray Photoelectron Spectroscopy (XPS)**, ***C. Mahoney***, *K.L. Steffens*, *A.J. Fahey*, *B.A. Benner*, National Institute of Standards and Technology, *R.T. Lareau*, Transportation Security Laboratory **INVITED**

Over the past decade, we at the National Institute of Standards and Technology have been working closely with the Department of Homeland Security to stop the threat of terrorist-based attacks in the form of explosives or explosive-based devices. Our program encompasses many different aspects of this threat, from development of measurement standards for trace explosives detection at airports, to the development and application of new metrology for the characterization these explosives. Here we present, to our knowledge, the first investigation into the application of surface analytical techniques, such as Secondary Ion Mass Spectrometry (SIMS) and X-Ray Photoelectron Spectroscopy (XPS) for the characterization and differentiation of plastic explosives. This particular work is focused on the characterization of composition C-4 explosives from several different regions.

Unlike traditional analytical techniques such as GCMS and/or LCMS, these powerful surface analytical tools allow for the simultaneous and direct characterization of <u>all</u> the components in C-4 (explosive components, additives, binders, contaminants etc.), as opposed to a partial analysis of extracted portions. Furthermore, the characterization of the explosive samples with ToF-SIMS and XPS will enable rapid identification of both organic and inorganic constituents as well as their characteristic isotopic abundances with excellent sensitivity. Most importantly, these techniques are well-suited for direct analysis of small explosive particulates collected directly in the field, and are already employed for homeland security applications that effect national policy.

11:20am **AS2-ThM11 Chemical Speciation of Engineered Nanoparticle Surface Chemistry with Secondary Ion Mass Spectrometry**, ***C. Szakal***, *R.D. Holbrook*, National Institute of Standards and Technology

As the sizes of nanostructures decrease, the surface-to-volume ratios increase immensely such that the smallest nanoparticles are theoretically seen by their surroundings as only the chemistry exposed on the surface and not the bulk of the nanoparticle interiors. We believe that the ability to track the surface chemistry of nanoparticles vs. size and vs. environmental exposures will show dramatically altered surface chemistry, and thus altered chemical reactivity of the nanoparticles. This concept has widely been suspected and/or believed to be true within the nanoparticle field, but experimentalists have yet to devise a standard approach at measuring what the surface chemistry is and to what extent that surface chemistry can be altered in real-world conditions. Since we are interested *only* in the surfaces of the nanoparticles and not necessarily the bulk, we have worked to develop a new paradigm for monitoring the surface chemistry of engineered nanoparticles with secondary ion mass spectrometry (SIMS). When kept in a static mode analysis, SIMS can be highly surface-sensitive to just a few nm, where other commonly employed techniques for measuring nanoparticle chemistries either cannot separate bulk vs. surface information, or only arrive at surface information indirectly. We will present progress made towards reaching our aims, including nanoparticle preparation considerations, sensitivity of SIMS to monitoring changes in the nanoparticle surfaces, and projections into the future of this methodology for such a purpose.

11:40am **AS2-ThM12 Complementary XPS and SEM/EDS Characterization of Gunshot Residue (GSR)**, *A.J. Schwoeble*, ***B.R. Strohmeier***, *J.D. Piasecki*, RJ Lee Group, Inc.

Discharged firearm cartridges produce unique microscopic particles referred to as gunshot residue (GSR). GSR is the product of combustion of the primer material. Depending on the type and brand of ammunition, GSR particles typically contain varying amounts of lead, barium, and antimony, along with one or more other elements, such as aluminum, silicon, phosphorus, sulfur (trace), chlorine, potassium, iron (trace), nickel, copper, zinc, zirconium, and tin. If particles containing lead, antimony, and barium are detected on a crime suspect's hands or clothing, it is taken as sufficient evidence that the person has either recently handled a discharged firearm, was present in the general vicinity of a weapon while it was discharged, or came in contact with a surface contaminated with GSR. Scanning electron microscopy (SEM) combined with energy dispersive X-ray spectroscopy (EDS) is the most commonly used technique for detecting the presence of GSR particles. GSR samples are collected from a suspect's hands and clothing using adhesives mounted on standard SEM sample stubs. SEM imaging is used to verify the characteristic size, shape, and morphology of GSR particles and EDS can identify the elemental composition of individual particles.

Determining the presence of lead, barium, and antimony fused together in a single particle having the correct morphology is all that is normally required for the positive identification of GSR. However, because of the high temperatures (~1,500-3,600 °C) and pressures (~14,000-65,000 psi) that result within 1 millisecond of discharging a firearm cartridge, highly complicated chemical interactions are likely to occur that will affect the chemical composition of the GSR particles. Because of its nanometer-scale sampling depth and the ability to provide detailed chemical state information, X-ray photoelectron spectroscopy (XPS) can provide important information regarding the surface chemistry of GSR; therefore, XPS offers potential as a complementary technique to SEM/EDS analysis. The aim of this investigation was to use XPS to gain further knowledge regarding the surface chemistry of GSR.

Authors Index

Bold page numbers indicate the presenter