Environmental Molecular Sciences Workshop
May 21, 2001

Richard Reeder (SUNY, Stony Brook)

Tony Lanzirotti (U. of Chicago)

This year's Environmental-Molecular Sciences Workshop was held as part of the National Synchrotron Light Source's Annual Users' Meeting on May 21, 2001. Organized by Tony Lanzirotti (GSECARS, U. Chicago) and Rich Reeder (Geosci. Dept., SUNY Stony Brook), this is the second in what is hoped will be an annual event. Eight speakers presented research conducted at beamlines at the NSLS. Doug Hunter (Savannah River Tech. Center) showed how interpretation of chemical processes in contaminated soils often requires both bulk- and micro-sample analysis. To illustrate this he presented bulk EXAFS (X23A2), microbeam XANES and XRF (X26A), and FTIR and Raman data on plutonium and chromium contaminated tuffs and uranium contaminated soils.

Don Sparks (Dept. of Plant and Soil Sci., U. Delaware) touched on the similar issue of how to relate field observations made for contaminated soils to molecular and atomic scale interactions. He presented data from zinc and arsenic contaminated sites, emphasizing that proper interpretation requires the use of multiple techniques such as EMPA, XRD, EXAFS (X11), and microbeam XRF and XANES (X26A).

Jay Brandes (Marine Sci. Inst., U. Texas-Austin) showed how soft x-ray transmission microscopy (X1A) is used to evaluate sources of carbon in marine environments. These samples, some collected at over 3400 meters depth in the ocean, are dominated by remnants of marine organisms and provide unique insights into the sources of organic carbon at these depths. He illustrated how sub-micron spatial resolutions are needed to precisely evaluate the composition of these environmental materials.

Jeff Gillow (Dept. of Environ. Sci., BNL) presented research on how bacterial organisms can affect the migration mechanisms of actinides in the environment. In particular, how colloidal mobilization by bacteria became an issue at the Waste Isolation Pilot Plant (WIPP) in NM. Based on SEM-TEM-EDS analyses, EXAFS results from X11, and STXM data from X1A, Jeff showed

that bacterial species such as Halomonas and Clostridium effectively complex uranium within their cell structure.

Murthy Vairavamurthy (Dept. of Environ. Sci., BNL) showed how x-ray absorption spectroscopy (X19A) is used to evaluate the role S and N in forming macromolecules and in driving organic matter transformations from bio- to geo-polymers. He demonstrated that catalysis and abiotic transformations are important mechanisms in these processes.

John Parise (Geosci. Dept., SUNY Stony Brook) presented a discussion of state-of-the-art developments in the application of micro-beam XRD to earth science materials (X26A). He demonstrated how such spatially resolved (10 micron) analyses can be coupled with simultaneous XRF and XANES analysis to provide a more complete understanding of the geochemical environment of a material.

Andreas Scheinost (Inst. of Terrestrial Ecology, ETH) presented data from a number of zinc contaminated sites and emphasized that spatially resolved XAS and XRF are almost a requirement to understanding the heterogeneous distribution of contaminants in soils. He demonstrated using principal component analysis on directly sampled materials and samples treated by selective sequential extraction that the zinc distribution in these soils reflects a diverse mineralogy at micron scale.

Lastly, Richard Osgood (BNL and Columbia U.) presented results that provide fundamental first-order data on the nature of the sub-surface transport of metal oxides by looking at reactions occurring at metal-oxide/water-interface model surfaces (Fe, Fe_2O_3 Fe_3O_4, etc.). Such minerals (e.g. hematite) are known to promote the reduction Cr^{6+} and dehalogenate compounds such as CCl_4. Combining a variety of analytical tools (UHVSTM/AFM, AES/SIMS, NEXAFS, and XPS) they were able to identify the reaction products formed on the metal surface and how these surface species are desorbed.

It's clear that the excellent turnout for this year's workshop emphasizes the need for ongoing interaction between environmental researchers in using synchrotron sourced facilities. *Virtually all the speakers emphasized the need to apply multiple analytical techniques in evaluating environmental problems. There was also a common feeling that there is a need for improved spatial resolutions in synchrotron based XRF, XAS, and XRD analysis.* Hopefully, future workshops will act to promote the exchange of new ideas, attract new environmental researchers to these facilities and provide a forum to stimulate innovations in techniques and methodologies.