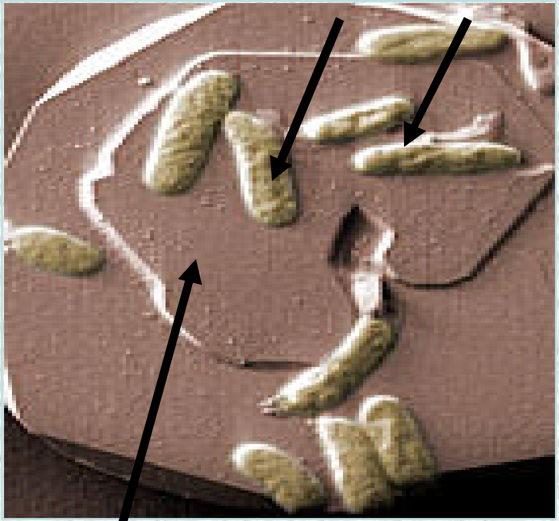
2004 APS Users Meeting Workshop

Future Directions in Synchrotron Environmental Science

Organizers: S. Sutton (U. Chicago), K. Kemner and S. Kelly (ANL-ER)

Microbe-Mineral Interactions

Shewanella



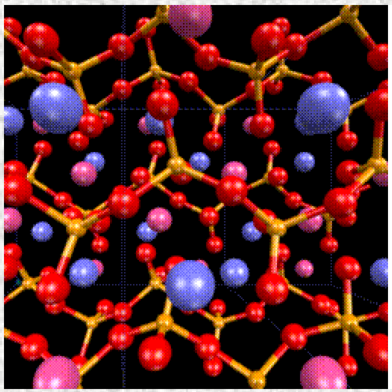
Tabular hematite (Fe_2O_3)

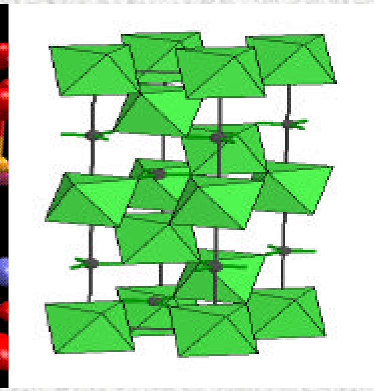
(J. Fredrickson, PNNL)

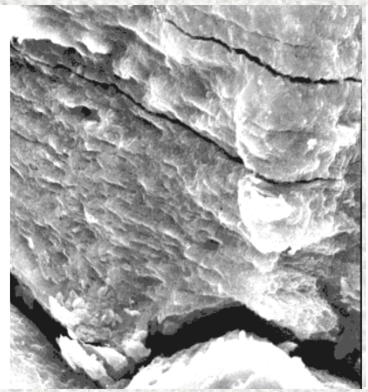
Remediation of Contaminated Groundwater

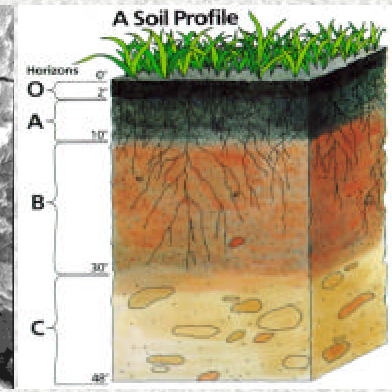
(Bangladesh; S. Fendorf, Stanford U.)

Atomic **Molecular** **Microscopic** **Macroscopic** **Field**









Atomic

- XRF
- XPS
- XAS

Requires synchrotron radiation.

Molecular

- XRD
- TGA
- FTIR
- DRS

Microscopic

- Enhanced Visual Analysis:
  1. SEM
  2. TEM
  3. AFM

Macroscopic

- Field Plots
- Equilibrium Studies
- Kinetic Studies
- Extractions

Field

- Visual/ Intuitive Insight
- Field Plots

K. Scheckel (EPA); Adaptation of Bertsch and Hunter, 1996.

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Future Directions in Synchrotron Environmental Science

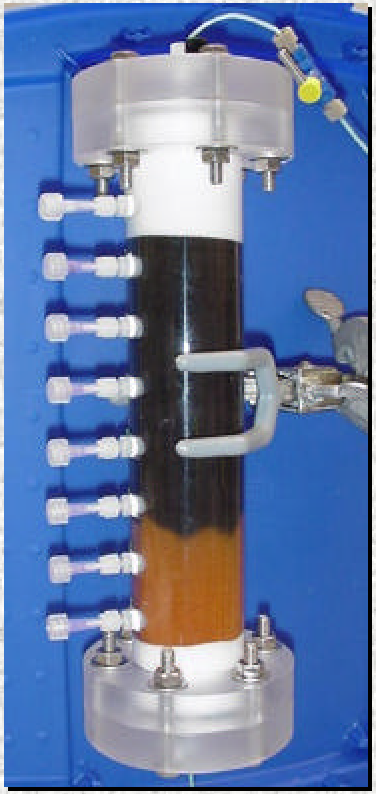
Agenda

Overview of Synchrotron Environmental Science	**Ken Kemner** (ANL)
How Do Metal-Reducing Bacteria Deal with Solid Phases?	**Jim Fredrickson** (Pacific Northwest National Laboratory)
Surface Complexation Models of Metal Cation Adsorption onto Bacterial	**Jeremy Fein** (University of Notre Dame)
Bioremediation of U Contaminated Subsurface Environments and the Role of Synchrotron-based X-ray Absorption Measurements	**Shelly Kelly** (Argonne National Laboratory)
Application of Synchrotron Radiation Based Techniques to the Biogenic Oxidation of Manganese	**Sam Webb** (Stanford University)
Environmental Science using the PNC-CAT Microprobes and Possible Future Directions	**Steve Heald** (Pacific Northwest National Laboratory)
Mineral-Water Interface Studies	**Tom Trainor** (University of Alaska)
Elemental, Chemical and Structural Characterization of Mineral-Water Interfaces with X-ray Scattering Techniques	**Paul Fenter** (ANL)
Correlating Metal Speciation in Soils to Risk	**Kirk Scheckel** (Environmental Protection Agency-Cincinnati)
Impact of Redox Disequilibria on Contaminant Transport and Remediation in Subsurface Systems	**Robert Ford** (Environmental Protection Agency-Oklahoma)
Resolving Biogeochemical Processes of Metals within Physically and Chemical Heterogeneous Media	**Scott Fendorf** (Stanford University)
Workshop Summary	**Paul Bertsch** (University of Georgia/SREL)

Scientific Topics

- Electron transfer reactions involving microbe-mineral interactions
- Bioremediation of reducible metals and radionuclides
- Metal binding mechanisms in microorganisms under varying chemical conditions.
- Molecular-level information on surface structure-reactivity relationships of hydrated mineral surfaces
- Sorption processes on mineral surfaces in presence of surface modifiers (water, biofilms and organics).
- Fate, transport and bioavailability of uranium in contaminated ground water plumes
- Microfracture localization of uranium from leaking high level waste tanks
- Remediation technology development: phytoremediation; reactive barriers; role of low abundance phases and preferential flow

Solid phase transformations

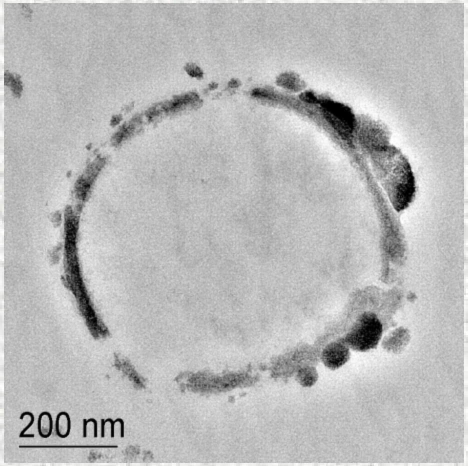


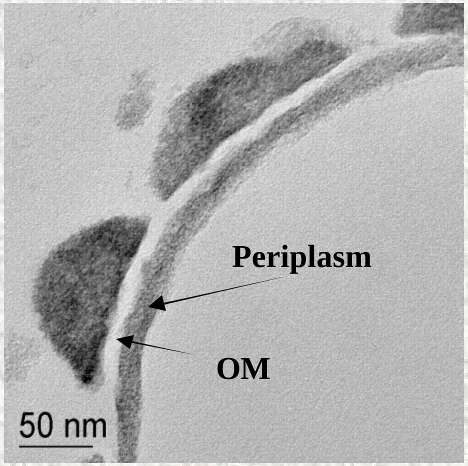
(S. Fendorf et al., Stanford)

Future Directions (Science)

- Define electron transfer mechanisms between microbes and minerals; cell wall chemistry
- Improved extrapolation of laboratory results to natural systems
- Improved understanding of coupled physical, biological, chemical processes in natural environments
- Expanded knowledge of mineral surface properties: bulk structures, compositions, orientations, natural solids
- Experimental tests of mechanistic predictive models of sorption
- Binding mechanisms of NOM/bacteria
- Impact of heterogeneous redox reactions on surface structure and reactivity
- Assessment of microscale heterogeneity in biogeochemical cycles
- Validation of macroscopic tests used to assess contaminant speciation, e.g. 'selective' extractions
- Reactivity of poorly crystalline materials, common in contaminated systems

Reduction of TcO^{4-} by MR-1 GSPD





J. Fredrickson, PNNL

Future Directions (Technical)

- Computational advances for fundamental modeling of organic and mineral structures and their chemical dynamics
- Advances in high resolution microscopies, spatially specific spectroscopies, and new imaging techniques
- Continued improvement in spatial resolution; easily varied beam-size from mm to nm
- Multiple-combined techniques in single instrument
- Quick or slew scanning for microspectroscopy
- More efficient detectors for improved detection limits
- Seamless integration of scattering and spectroscopy
- Improved ability for surface studies on small samples/select regions using microbeam techniques
- Dedicated ancillary facilities for specimen preparation and characterization

Study of Live Plant at Sector 20

K. Scheckel, EPA

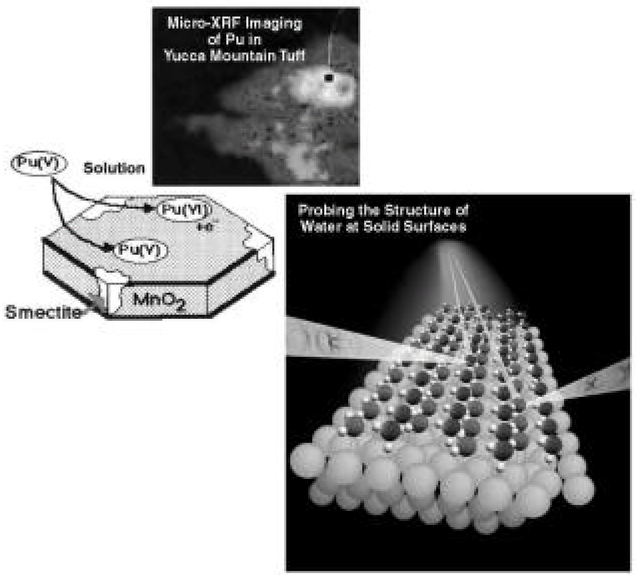
Points from Workshop Summary and Discussion

- Synchrotron-based X-ray techniques have emerged as very important tools for examining complex environmental samples to provide insights into the hydrobiogeochemical processes that control the fate, transport, and bioavailability of contaminants and nutrients.
- Synchrotron environmental science (SES) user community has experienced dramatic growth over the past decade and the future growth should significantly increase the APS user community.
- SES user community has specialized requirements for instrumentation and sampling preparation/characterization apparatus.
- Nature of the samples can vary significantly as do requirements for handling and preparing these samples under carefully controlled environmental conditions.
- These specialized needs and flexibility requirements suggest science-focused facilities/beamlines should be considered in addition to more distributed resources.

SLAC-R-704

2003 Report of EnviroSync – A National Organization of Environmental Science Users of Synchrotron Radiation Sources

Molecular Environmental Science: An Assessment of Research Accomplishments, Available Synchrotron Radiation Facilities, and Needs



Prepared in part for the Department of Energy under contract DE-AC03-76SF00515

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Stanford Synchrotron Radiation Laboratory
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MOLECULAR ENVIRONMENTAL SCIENCE:
An Assessment of Research Accomplishments, Available Synchrotron Radiation Facilities, and Needs

Prepared on behalf of *EnviroSync* by

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Executive Summary

Synchrotron-based techniques are fundamental to research in *Molecular Environmental Science* (MES), an emerging field that involves molecular-level studies of chemical and biological processes affecting the speciation, properties, and behavior of contaminants, pollutants, and nutrients in the ecosphere. These techniques enable the study of aqueous solute complexes, poorly crystalline materials, solid-liquid interfaces, mineral-aqueous solution interactions, microbial biofilm-heavy metal interactions, heavy metal-plant interactions, complex material microstructures, and nanomaterials, all of which are important components or processes in the environment. Basic understanding of environmental materials and processes at the molecular scale is essential for risk assessment and management, and reduction of environmental pollutants at field, landscape, and global scales.

One of the main purposes of this report is to illustrate the role of synchrotron radiation (SR)-based studies in environmental science and related fields and their impact on environmental problems of importance to society. A major driving force for MES research is the need to characterize, treat, and/or dispose of vast quantities of contaminated materials, including groundwater, sediments, and soils, and to process wastes, at an estimated cost exceeding 150 billion dollars through 2070. A major component of this problem derives from high-level nuclear waste. Other significant components come from mining and industrial wastes,

EnviroSync Recommendations

- ***Increase Operations Funding for Existing Beam Line Stations***
- ***Increase Beam Line Station Availability for MES Activities***
  - *Redirect Existing Beam Line Stations*
  - *Plan for New Beam Line Stations*
  - *Enhance Access to Existing Innovative Beam Line Stations*
- ***Increase Funding for Essential Equipment and Sample Handling Facilities***
- ***Survey the Environmental Science Community to Determine Highest Priorities and Needs***