GSECARS Surface, Interface, and Ambient-Pressure Diffraction Program

Prepared by Peter Eng (PI), Joanne Stubbs
GeoSoilEnviroCARS, The University of Chicago

The Surface, Interface, and Ambient-Pressure Diffraction (SIA) program at GSECARS focuses on molecular-scale determination of crystal termination structure, mineral interactions with aqueous solutions and solutes, adsorbate conformation, and mineral reactivity. It is jointly funded by NSF-EAR-IF and DOE-BES Geosciences. The program operates in the 13-BM-C and 13-ID-C stations at the Advanced Photon Source (APS). The program in the 13-BM-C station shares beam time, x-ray optics and instrumentation with the COMPRES-GSECARS PX^2 Partnership. The program in the 13-ID-C station shares beam time, x-ray optics and instrumentation with the GSECARS Large Volume Press (LVP) and Diamond Anvil Cell (DAC) programs.

For more than twenty years, users of the SIA program have used x-ray scattering and spectroscopic techniques to explore the manner in which adsorbates (e.g., lead, chromium, arsenic) bind to mineral surfaces in efforts to predict their fate in natural waters, to discover molecular-scale reaction mechanisms, and to investigate the influence of chemical, thermal, and redox stimuli on mineral-water interfacial reactions. Throughout our history we have trained numerous students, postdoctoral scholars, and other researchers in the application of x-ray methods to mineral-water interactions. In addition to providing one-on-one training at the beamline, we lead workshops and tutorials, and share our expertise and passion for science with middle and high school students via a variety of educational programs, actively seeking to engage and excite the next generation of the STEM workforce.

The present proposal highlights recent program accomplishments, including the development of sample environments that enable the determination of atomic-scale structures of mineral-water interfaces from crystals with surfaces that are smaller (< 300 microns) than have ever been measured as well as controlled mineral redox reactions mediated by in situ electrochemistry. It further highlights upgrades in-progress to the instruments used to make these measurements, which will soon enable richer and more rapid exploration of interfacial phenomena than previously possible.

Our plans for the next several years include:

- Development of advanced sample environments, including those that facilitate interfacial measurements conducted in flowing solutions and under hydrothermal conditions
- Advancing reciprocal space mapping capabilities for the exploration of complex, heterogeneous mineral-water interfaces
- Exploiting the APS-U upgrade to bring the power and promise of coherent x-ray scattering to mineral-water interface problems, including nanoparticle reactivity and the measurement of complex interfacial morphologies and chemistries
- Enhancing our data analysis programs by improving ease of use, and providing advanced model building tools that include chemical and steric constraints

The SIA program is partially supported by the NSF-EAR-IF program and partly by the DOE Geosciences program. We propose to continue at our present level of about 1.1 FTE support from this new NSF proposal.