

X-ray Method Images Ions at Interface

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A team led by Northwestern University researchers at the U.S. Department of Energy's Argonne National Laboratory have taken the guesswork out of interfacial structure determination. The researchers are **the first to show that three-dimensional images of ion site distributions at the mineral-water interface can be directly visualized using a technique called X-ray standing wave (XSW) imaging.** Their findings, published in the journal Surface Science Letters, demonstrate a new capability for revealing complex reactions at mineral-water interfaces that previously could be understood only through more indirect approaches.

This research builds on earlier work done by Michael Bedzyk, an author on the paper and a professor of materials science and engineering at Northwestern, and his colleagues. Using XSW to determine structures of interest, they initially imaged impurity atoms in mica -- a capability that, for example, will be useful in the emerging area of optoelectronics -- and then moved on to imaging tin atoms on the surface of germanium (a semi-metallic element). Both projects were the first such demonstrations using XSW imaging, which produces images with sub-angstrom resolution (less than one-tenth of a nanometer).

The researchers' long-term goal is to learn how to use X-rays to "see" geochemical processes in action at the molecular level. Solid-liquid interface structure is essential to many natural and technological processes. The interaction of mineral surfaces with fluids controls rock weathering, evolution of petroleum reservoirs and ore deposits, and the transport and remediation of contaminants in groundwater.

“Environmental scientists and engineers want to understand how toxic elements are transported in groundwater, and the chemistry essential to this process is happening at the surface,” said Bedzyk, an XSW expert who has applied the technique to many different problems. “XSW also allows us to study molecular self-assembly where molecules naturally assemble to form complex nanostructures. Understanding how that growth proceeds atom by atom will help in the design of future kinds of nanoscale devices.”

XSW, in contrast to X-ray crystallography, measures both the amplitude and phase information that completely describe the molecular-scale structure of interest. In standard crystallography only the amplitudes can be measured and consequently an elaborate approach is needed to determine the structure. The XSW imaging approach allows scientists to streamline the tedious process of structure determination, which previously took weeks or months to complete. Data acquisition and analysis now can be completed in less than 24 hours.

The Surface Science Letters research was conducted at the Basic Energy Sciences Synchrotron Radiation Center at the Advanced Photon Source (APS). The APS, which produces the most brilliant X-rays for research in the Western Hemisphere, is ideal for this type of research.

Authors on the report, in addition to Bedzyk, are Zhan Zhang of Northwestern University (lead author), Likwan Cheng and Paul Fenter of Argonne, Neil Sturchio of the University of Illinois at Chicago and Argonne, Michael Machesky of the Illinois Water Survey and David Wesolowski of Oak Ridge National Laboratory.

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The original news release is available [here](#).

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