

**FA5-MS39-T01****Real-Time X-Ray Studies of the Effect of Chemical Transients on Oxide Thin Film Surface Structure.**

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Modifying the chemical environment (e.g. the oxygen partial pressure) above a complex oxide can induce significant structural and electronic changes in its surface. Surface x-ray scattering studies are uniquely capable of probing the structure and dynamics of these rearrangements because of their ability to penetrate into complex and near-atmospheric pressure environments with time resolution down to nanoseconds, and with sub-micron spatial resolution. We are using these capabilities to explore basic mechanisms of materials synthesis and processing. In this talk, I will present recent results from our research programs at the Advanced Photon Source, including studies of chemical switching of ferroelectric PbTiO<sub>3</sub> where surface structure is strongly coupled to the polarization structure of the entire film, and high temperature structure and segregation in complex oxides such as La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub>. Looking to the future, spatially coherent x-ray sources such as free-electron lasers offer spectacular performance gains over current x-ray sources. I will discuss the fundamental knowledge that new and improved x-ray techniques using these new sources may yield, and how that knowledge might enable creation of high-performance materials with unique properties. Work including use of the Advanced Photon Source and Center for Nanoscale Materials is supported by U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract DE-AC02-06CH11357.

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**FA5-MS39-T02****Surface X-ray diffraction on mineral surfaces in environmental conditions.** Uta Magdans, *Department of Geology, Mineralogy and Geophysics, Ruhr-*

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Surfaces reactions and interactions of minerals play an important role in many geological and environmental, as well as in industrial processes, e.g. weathering, biomineralization or heterogeneous catalysis. Most of these surfaces are well characterized in UHV conditions with experimental techniques like STM, XPS or LEED. But are these results comparable to "real" environmental conditions, with ambient temperature and pressure, including the presence of water in the atmosphere?

Surface X-ray diffraction techniques carried out with synchrotron radiation provide an excellent tool to obtain information about the surface and interface structure of minerals in dry and humid atmosphere. With crystal truncation

rod diffraction studies we observed the formation of an laterally ordered hydration layer on the (104) surface of calcite (CaCO<sub>3</sub>) and the (100) fluorapatite (Ca<sub>5</sub>(PO<sub>4</sub>)<sub>3</sub>F) surface with increasing humidity. Both surfaces showed no reconstruction, but a bulk terminated, relaxed surface structure, respectively [1,2].

Crystal truncation rod scattering experiments allow also to determine the water-mineral interface structure of the completely hydrated mineral surface. Here the calcite (104) and the fluorapatite (100) surface were covered with a water film, which leads to a 1-2 monolayers thick ordered water layer above the topmost surface layers, stabilizing dangling bonds and forming a strong hydrogen bond network [3,4].

With the mineral surface in contact with an aqueous solution of small molecules, e.g. simple amino acids like glycine and proline, we were able to resolve the water-molecule-mineral interface structure with surface X-ray diffraction on calcite, fluorapatite and pyrite surfaces [3,5]. This provides a model system to understand the influence of small biomolecules on the formation of biominerals or, as in the case of pyrite, insight in the function of mineral surfaces serving as templates during the emergence of complex biomolecules in the prebiotic world.

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**FA5-MS39-T03****X-ray investigation of the morphology of DCV6T-Bu<sub>4</sub> films for Organic Solar Cells.** Alexandr A. Levin<sup>a</sup>, Marieta Levichkova<sup>a</sup>, Dirk Hildebrandt<sup>b</sup>, Andre Weiss<sup>b</sup>, Marina Klisch<sup>b</sup>, Chris Elschner<sup>a</sup>, David Wynands<sup>a</sup>, Martin Pfeiffer<sup>b</sup>, Karl Leo<sup>a</sup>, Moritz Riede<sup>a</sup>.

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Dicyanovinyl-substituted sexithiophene with four butyl chains (DCV6T-Bu<sub>4</sub>), C<sub>32</sub>H<sub>10</sub>N<sub>4</sub>S<sub>6</sub>-(C<sub>4</sub>H<sub>9</sub>)<sub>4</sub>, is a new promising photoactive material for organic solar cells. The influence of the film thickness (3.5 nm to 50 nm), the substrate temperature (30 °C or 90 °C) during the film deposition, and the kind of buffer underlayer on the atomic structure, microstructure, and film morphology of the DCV6T-Bu<sub>4</sub> neat layers is investigated by means of X-ray diffraction (XRD) and X-ray reflectivity (XRR) methods. A Si wafer or a Si wafer covered by a 15 nm-thick buffer underlayer of fullerene, C<sub>60</sub>, or 9,9-Bis[4-(N,N-bis-biphenyl-4-yl-amino)phenyl]-9H-fluorene (BPAPF), C<sub>73</sub>H<sub>52</sub>N<sub>2</sub>, is used as substrate.

The crystalline nature and ordered molecular arrangement of the DCV6T-Bu<sub>4</sub> films are proven by XRD down to 6 nm film thickness. The films grown on heated substrates (90 °C) are characterized by a better crystallinity. With increasing substrate temperature from 30 °C to 90 °C, the size of the DCV6T-Bu<sub>4</sub> crystallites in direction perpendicular to the film