3D imaging of geological materials using x-ray diffraction and spectroscopy

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Geological materials typically exhibit homogeneous mineralogy, such as chemical or structural variations, which can vary on the order of microns to millimeters. The capabilities of high-energy synchrotron x-rays using a focused microbeam to probe these materials can be exploited to study such homogeneities. By rastering a specimen using the micron-sized beam, a two-dimensional map of diffraction and spectroscopic data can be collected. Three-dimensional tomographic datasets can be created by both rastering and rotating the specimen in the beam.

Combined techniques such as these are incredibly valuable for making connections between chemical state and mineralogy in homogenous materials. The identified chemistry can provide clues to the possible minerals within a given sample. Information from the scattering data can be used to extract crystal structure information throughout the specimen volume, allowing for the identification of new and unknown phases within the volume, characterizing orientation distribution, and possibly even describing the strain state of the material.

Our group is developing software tools to collect and analyze data from these combined techniques in order to create diffraction and fluorescence tomographic reconstructions. The LARCH [1] software suite has been extended to include x-ray diffraction, partially powered with pyFAI [2], and tomography capabilities, using tomoPY [3]. This talk will discuss the collected datasets, as well as the current software and data analysis capabilities.

[1] Newville (2013) J. Phys.: Conf. Ser. 430 012007
[2] Kieffer & Karkoulis (2013) J. Phys.: Conf. Ser. 425 202012
[3] Gursoy, et al. (2014) J. Sync. Rad. 21 1188