Compressive signal collection for dynamic tabletop X-ray absorption spectroscopy (XAS)

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X-ray Absorption Fine-Structure Spectroscopy (XAFS) is a powerful analytical technique, which works with almost any sample environment, as compared to X-ray crystallography, for obtaining elemental and chemical information in many fields such as biosciences, material sciences, catalysis and physical chemistry.[1,2] XAFS utilizes a large bandwidth radiation that is tuned sequentially to capture the entire spectrum where the resolution is dependent on the monochromator. The entire scanning of certain samples can take relatively long times. High brightness, essential for enough sensitivity, can be destructive for certain samples. Time resolved XAFS needs complex optical setups and fast signal processing techniques to resulting in a data deluge. Source features are obtained at synchrotron beamlines. Few of these exist worldwide, with limited access due to large amount of proposals.

Ideally, one would like to have a single shot acquisition of the entire spectrum, where the entire scanning should be faster than the chemical reaction being studied. Furthermore, the source should at low sample damage intensity, without sacrificing information and the required resolution should be close to few meV. Advantageously, this method should be available in each laboratory.

Aim of this study was to develop a data processing method, which can match and compliment as much as possible such requirements. Compressed Sensing (CS) is a well-known procedure in signal processing used to acquire and reconstruct undersampled data sets without losing any important information about the signal. Taking advantage of the sparsity of the spectral signal in a fixed basis and when sampled randomly, the data acquisition can be dynamic, where in one case the sampling rate is varied or in the second case the acquisition time. Aided by convex optimization solvers, faster and reliable data acquisition is possible with competent data reconstruction.

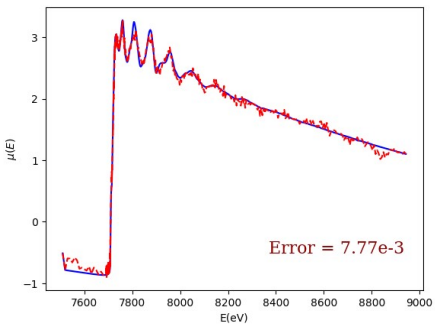

Figure 1: Reconstructed signal (red) vs reference signal (blue). Comparison for a Co foil, which is sampled randomly at 30%.

This research shows as a proof of concept, the advantages and limitations of the compressed sensing technique for XAFS data acquisition using a laboratory X-ray source. The results from many different samples tested with the code show that even with as less as 30 % of data sampling, the error for reconstruction of the XAFS spectrum is less than or equal to 1%. Example of Co foil is shown in Figure 1. The reconstructed raw data also translates reliably for K-space and R-space analysis. A big advantage is pre-emptive studies of unknown samples. The limitation is more peaks in the spectral signal means more sampling is required for complex signals. Therefore, compressed sensing for XAFS is useful for fast and reliable data acquisition with low noise, within a few minutes on tabletop.

[1] M. Newville, *Rev. Mineral. Geochem.* **2014**, 78, 33-74.
[2] S. Calvin, XAFS for Everyone, CRC press, **2013**.