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Compressive signal collection for dynamic XAFS in the home lab

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X-ray Absorption Spectroscopy (XAFS) is a widely used powerful technique for obtaining elemental and chemical information in many fields such as biosciences, material sciences, catalysis and physical chemistry. XAFS utilizes a large bandwidth radiation that is tuned sequentially to capture the entire spectrum where the resolution is dependent on the monochromator bandwidth. The entire scanning of certain samples can take relatively long times and high brightness is essential for enough sensitivity. Additionally, time resolved XAFS need complex optical setups and fast signal processing techniques to resulting in a data deluge. Few of such synchrotron sources 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 show operate at low 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 method, which can match as much as possible such requirements. The method mentioned relies on efficient data processing, where it is possible to compensate for the reduced complexity of the instrumentation used, with more advanced data treatment. Compressed Sensing (CS) is a well-known procedure in signal processing used to acquire and reconstruct under-sampled data sets without losing any important information about the signal. Taking advantage of the sparsity of spectral signal, 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 signal processing techniques, faster and reliable data acquisition is possible with competent results.
This research shows as a proof of concept, the advantages and limitations of the compressed sensing technique and puts forward an experimental setup to acquire, in real time, XAFS signals using a laboratory X-ray source and the compressed sensing algorithm. The results from different samples show that the percentage of the acquired data directly corresponds to the accuracy of reconstruction of XAFS signal, more sampling results in more accurate reconstruction. Additionally, even with as less as 25 % of sampling , the error for reconstruction of the XAFS spectrum for different samples is less than or equal to 1% which shows with acquiring only a few amount of components, XAFS data can be accurately reconstructed for analysis.

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