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Full Length Article

Analysis of extended X-ray absorption fine structure (EXAFS) data using artificial intelligence techniques

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ABSTRACT

We have addressed the issue of improper and unreliable analysis of materials characterization data by developing an artificial intelligence based methodology that can reliably and more efficiently analyze experimental results from extended X-ray absorption fine structure (EXAFS) measurements. Such methods help address growing reproducibility problems that are slowing research progress, discouraging the quest for research excellence, and inhibiting effective technology transfer and manufacturing innovation. We have developed a machine learning system for automated analysis of EXAFS spectroscopy measurements and demonstrated its effectiveness on measurements collected at powerful, third generation synchrotron radiation facilities. Specifically, the system uses a genetic algorithm to efficiently find sets of structural parameters that lead to high quality fits of the experimental spectra. A human analyst suggests a set of chemical compounds potentially present in the sample, used as theoretical standards. The algorithm then searches the large multidimensional space of combinations of these materials to determine the set of structural paths using the theoretical standards that best reproduces the experimental data. The algorithm further calculates a goodness of fit value from the suggested standards that can be used to identify the chemical moieties present in the measured sample.

1. Introduction

A growing body of unreliable and irreproducible research results has been (and continues to be) published because they rely upon improper materials characterization analysis [1]. The presence of these unreliable results can lead researchers to waste time and resources to develop new materials based on these problematic analyses. A critical cause of this problem is the relatively small number of characterization experts who can accurately analyze measurement data. A vast number of datasets on materials, surfaces, and interfaces are generated every day, and only a small fraction can be analyzed by characterization experts. This bottleneck can be addressed by harnessing modern computational techniques to automate the analysis and make the process more reliable and reproducible.

Another benefit of automating data analysis, especially with large, complex datasets commonly found in *in situ* and *operando* measurements, is the ability to more expediently process and disseminate research results. By implementing a more efficient approach, a greater number and variety of new results can be readily added to the body of knowledge for new materials, thus facilitating materials discovery. Here, we outline an artificial intelligence method for processing extended X-ray absorption fine structure (EXAFS) data.

There are a number of potential methods for using artificial intelligence to analyze EXAFS data. Two strong examples of these methods are neural networks and evolutionary algorithms. Neural network approaches have been used in EXAFS analysis to identify local atomic

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