APS Scientific Computation Seminar Series

Speaker: Jeff Terry
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Title: Analysis of Synchrotron Extended X-ray Absorption Fine Structure (EXAFS) Data Using Artificial Intelligence

Date: Monday, July 20, 2020

Time: 1:00 p.m.

Location: https://bluejeans.com/655353553

Hosts: Nicholas Schwarz, Mathew Cherukara, and Jessica McChesney

Abstract:

A growing body of unreliable and irreproducible research results have been published because they rely upon improper materials characterization analysis [1]. New results build on old. Thus, when previous results cannot be trusted, the entire scientific process is hampered. Researchers have to waste time and resources on doomed attempts to do research and develop processes based on incorrect assumptions. One of the causes of this is that there are limitations on the number of characterization experts who can analyze data collected on the vast number of materials, surfaces, and interfaces developed every day. We have addressed this problem by developing artificial intelligence based methodology that can be utilized to reliably analyze experimental results from Extended X-ray Absorption Fine Structure (EXAFS) measurements. This development will help to address the reproducibility problems that slow research progress and inhibit effective tech transfer and manufacturing innovation in these scientific disciplines.

A machine learning approach was applied to the analysis of extended X-ray absorption fine structure (EXAFS) spectroscopy measurements collected using a synchrotron radiation facility. Specifically, a genetic algorithm was developed for fitting of the measured spectra to extract the relevant structural parameters. The current approach relies on a human analyst to suggest a potential set of chemical compounds that may be present. The algorithm than attempts to determine the best structural paths from these compounds that are present in the experimental measurement. The automated analysis looks for the primary EXAFS path contributors from the potential compounds. It calculates a goodness of fit value that can be used to identify the chemical moieties present.

Reference:

[1] Linford, M. R.; Smentkowski, V. S.; Grant, J. T.; Brundle, C. R.; Sherwood, P. M.; Biesinger, M. C.; Terry, J.; Artyushkova, K.; Herrera-Gomez, A.; Tougaard, S.; et al., Proliferation of Faulty Materials Data Analysis in the Literature, *Microscopy and Microanalysis* 2020, 26, 1-2.