JVST A
Journal of Vacuum Science & Technology A

ARTICLE

pubs.aip.org/avs/jva

Analysis of x-ray emission spectroscopy (XES) data using artificial intelligence techniques included in the XES Neo package

Cite as: J. Vac. Sci. Technol. A **43**, 043411 (2025); doi: 10.1116/6.0004326
Submitted: 18 December 2024 · Accepted: 19 March 2025 ·
Published Online: 9 June 2025

Alaina Humiston,[1,2] Miu Lun Lau,[3] Tim Stack,[1] Evan Restuccia,[1] Alberto Herrera-Gomez,[4] Min Long,[3] Daniel T. Olive,[2] and Jeff Terry[1,5,a)]

AFFILIATIONS

[1]Department of Physics, Illinois Institute of Technology, 3101 South Dearborn Street, Chicago, Illinois 60616
[2]Materials Science and Technology Division, Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, New Mexico 87545
[3]Department of Computer Science, Boise State, 1910 W University Dr. Boise, Idaho 83725
[4]CINVESTAV-Unidad Queretaro, Libramiento Norponiente No. 2000, Fracc. Real de Juriquilla., Santiago de Querétaro C.P. 76230, Qro., Mexico
[5]Department of Mechanical, Materials, and Aerospace Engineering, Illinois Institute of Technology, 3101 South Dearborn Street, Chicago, Illinois 60616

Note: This paper is part of the Special Topic Collection on Artificial Intelligence and Machine Learning for Materials Discovery, Synthesis and Characterization.

[a)]**Author to whom correspondence should be addressed:** terryj@iit.edu

ABSTRACT

We have developed an artificial intelligence tool, XES Neo, for fitting x-ray emission spectroscopy (XES) data using a genetic algorithm. The Neo package has been applied to extended x-ray absorption fine structure [Terry *et al.*, Appl. Surf. Sci. **547**, 149059 (2021)] as well as Nanoindentation data [Burleigh *et al.*, Appl. Surf. Sci. **612**, 155734 (2023)] and is in development for x-ray photoelectron spectroscopy data. This package has been expanded to the fitting of XES data by incorporating basic background removal methods (baseline and linear) optimized simultaneously with peak-fitting using the active background approach, as well as the peak shapes Voigt, and an asymmetrical Voigt, known as the Double Lorentzian. The fit parameters are optimized using a robust metaheuristic method, which starts with a population of temporary solutions known as the chromosomes. This population is then evaluated and assigned a fitness score, from which the best solution is then found. Future generations are created through crossover of the best sets of parameters along with some random parameters. Mutation is then done on the new generation using random perturbations to the chromosomal parameters. The population is then evaluated again, and the process continues. The analyzed data presented here are available in the corresponding XESOasis discussion forum (https://xesoasis.org/ai_posted).

I. INTRODUCTION

A growing body of unreliable and irreproducible research results has been (and continues to be) published due to improper analysis of materials' characterization data.[1] These unreliable analyses can misguide researchers, leading to wasted time and resources in developing new materials based on inaccurate conclusions. One of the primary causes of this issue is the limited number of experts capable of accurately interpreting complex materials' characterization data. With new advancements in instrumentation[2,3] making x-ray emission spectroscopy (XES) data collection possible outside of synchrotron facilities, an increase in quantities of XES datasets is expected. However, only a small fraction of data can be analyzed by characterization specialists, possibly creating a critical bottleneck in the scientific discovery process.