AKPIK 6: AI Methods for Materials Science

Time: Thursday 16:30–18:00 Location: H5

AKPIK 6.1 Thu 16:30 H5

Bayesian Optimization for High-Resolution Transmission Electron Microscopy — •Xiankang Tang[1], Lei Jin[2], Yixuan Zhang[1], Rafal Dunin-Borkowski[2], and Hongbin Zhang[1] — [1]Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany — [2]Ernst Ruska-Centrum für Mikroskopie und Spectroskopie mit Elektronen, FZ Jülich, 52428 Jülich, Germany

Advances in machine learning technologies make it possible to automatize material characterizations, indispensable for the near-future implementation of autonomous experimentation for solid-state materials. High-resolution transmission electron microscopy (HRTEM) allows the study of the atomic structure of solid materials with sub-Angstrom resolution. By matching experimental and simulated images, unknown experimental parameters and crystal structures can be determined. However, this process entails strong domain expertise and can be time-consuming. In this work, we implement a Bayesian optimization-based approach to automatize the image analysis processes. Combined with some prior information, such as the experimentally measured aberration, the 3D crystal structure of the specimen can be reconstructed from a single HRTEM image. Specifically, by defining the mean square error(MSE) of pixel intensity values between experimental and simulated images, our method effectively captures both global and local image features. This approach not only achieves an exact match in absolute image contrast but also identifies unknown experimental parameters, optimizes atomic positions, and reveals surface morphology at atomic resolution.

AKPIK 6.2 Thu 16:45 H5

Synthetic Data Generation for Enhanced Segmentation of Electron Microscopy Images — •Amir Omidvarnia[1], Ali Ghaznavi[2], Junbeom Park[1], Shibabrata Basak[1], and Simone Köcher[1] — [1]Institute of Energy Technologies - Fundamental Electrochemistry (IET-1), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — [2]Federal Institute for Materials Research and Testing (BAM), 12205 Berlin, Germany

Monitoring structural changes in materials via operando electron microscopy (EM) is crucial for understanding the material's changes under operating conditions, which directly impacts its durability and performance. However, accurate segmentation of features such as cracks or pores in EM time-series data requires extensive labeled datasets, which are challenging to produce due to the labor-intensive, subjective nature of manual annotation. Our research addresses this limitation by exploring different synthetic data generation techniques that can effectively supplement scarce annotated data and improve segmentation outcomes. We evaluate multiple synthetic image generation approaches to enhance the training dataset for U-Net models aimed at segmenting EM time-series data: (1) deep convolutional generative adversarial networks (DCGAN) to produce realistic textures; (2) time-varying image synthesis that mimics the temporal development of features and introduces artificial features to simulate structural imperfections; and (3) standard data augmentation methods. These methods are evaluated in generating training data for EM image segmentation from a limited set of EM images.

AKPIK 6.3 Thu 17:00 H5

Neural Networks in Surface Crystallography: A New Paradigm for GIWAXS Analysis — •Erwin Pfeiler[1], Vladimir Starostin[3], Alexander Hinderhofer[3], Roland Resel[2], Frank Schreiber[3], and Stefan Kowarik[1] — [1]University of Graz, Austria — [2]TU Graz, Austria — [3]University of Tübingen, Germany

Thin film materials are essential to modern technology, with grazing incidence X-ray diffraction (GIWAXS) being the primary method for resolving their crystal structure. However, the current data analysis process is often slow and labor-intensive, frequently requiring more time and resources than the GIWAXS measurements themselves. Accelerating this bottleneck is critical for enabling automated materials discovery.

In this work, we present an AI-driven approach utilizing neural networks to streamline and enhance GIWAXS analysis. Our model predicts unit cell dimensions (a, b, c) and angles (α, β, γ) directly from the positions of Laue reflections. Additionally, it identifies the Miller indices of the contact plane, providing insights into the film texture.

Using both simulated GIWAXS data and real-world examples, we demonstrate the neural network's potential to significantly accelerate the analysis process, delivering accurate structural predictions with sub 0.01 Å precision.

AKPIK 6.4 Thu 17:15 H5

Reflectivity Analysis with AI: The LISA Data Pipeline at P08/DESY — •Julia Kobus[1,2], Lukas Petersdorf[1,2], Svenja Hövelmann[1,2], Alexander Hinderhofer[3], Vladimir Starostin[3], Chen Shen[4], Florian Bertram[4], Linus Pithan[4], Frank Schreiber[3], and Bridget Murphy[1,2,4] — [1]Institute of Experimental and Applied Physics, Kiel University, Leibnizstr. 19, 24118 Kiel, Germany — [2]Ruprecht-Haensel Laboratory, Olshausenstr. 40, 24098 Kiel, Germany — [3]University of Tübingen, 72076 Tübingen, Germany — [4]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany

We present a data analysis pipeline that is under development within TA3 of DAPHNE4NFDI for the LISA instrument at the P08 beamline at DESY. This pipeline is adapted from the development on solid surface XRR AI analysis to be used for liquid surfaces and interfaces. The pipeline aims at performing data reduction and subsequent analysis for reflectivity measurements using AI-based models. This approach increases measurement efficiency by processing data in real time, allowing flexible adjustments during the experiment and providing immediate insights. This will help users make better-informed decisions for subsequent measurements. The pipeline also will make advanced data analysis accessible to less experienced users. Our work will demonstrate the potential of AI to transform experimental workflows and data interpretation, and provides a blueprint for similar developments in the scientific community.

AKPIK 6.5 Thu 17:30 H5

Prediction of Infrared Spectra of organic molecules with Active Learning — •Gusein Bedirkhanov[1], Nitik Bhatia[1], Ondrej Krejci[2], and Patrick Rinke[1,2] — [1]Department of Physics, Technical University of Munich, Germany — [2]Department of Applied Physics, Aalto University, Finland

Infrared (IR) spectroscopy is a valuable tool for understanding catalytic processes, but interpreting experimental spectra is challenging due to the strong influence of the species environment. Ab initio molecular dynamics (AIMD) offers accurate theoretical spectra, accounting for anharmonic effects, but at a high computational cost. Machine-learned interatomic potentials (MLIPs), such as MACE [1], provide an alternative to AIMD, enabling accurate and fast IR spectra predictions. To reduce the amount of training data, we have established the active learning method PALIRS [2] (a Python-based active learning code for infrared spectroscopy). PALIRS predicts IR spectra of organic molecules essential in catalytic processes accurately, with peak positions matching experiment within 20cm^{-1}. We aim to further improve the efficiency of PALIRS, using only a hundredth of DFT data in comparison with AIMD, through optimization of MACE training strategies. We will inspect various combinations of transfer learning and conventional iterative training to find the ideal match between training time and final MLIP accuracy.

[1] I. Batatia *et al.*, Adv. Neural inf. Process. Syst. (2022).
[2] N. Bhatia *et al.*, GitHub (2024), `gitlab.com/cest-group/PALIRS`

AKPIK 6.6 Thu 17:45 H5

Towards AI-assisted high-throughput thin film research workflow — •Dmitry Lapkin, Roody Nasro, Constantin Völter, Valentin Munteanu, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — University of Tübingen

The compositional optimization of new materials necessitates the high-throughput screening of a multitude of compositions, which must be investigated to elucidate the non-linear and non-monotonic structure-property-composition dependencies. In this regard, data-driven material science enables researchers to accelerate the identification of new materials with desired properties for specific applications by efficiently exploring vast material spaces. Such high-throughput data-driven studies comprise two key elements: the combinatorial preparation of suitable sample libraries spanning wide compositional ranges, and the high-throughput screening of the structure and properties of

the synthesized samples.

In this work, we present a complete workflow for high-throughput studies of thin films. A specially designed vacuum deposition chamber enables the production of gradient thin films suitable for high-throughput screening. Surface-sensitive X-ray scattering methods available at modern X-ray sources comprise a convenient tool for resolving the thin film structure with ultimate resolution and high speed, while the developed AI-based approaches provide on-the-fly analysis of the collected X-ray scattering data.