ELEMENTAL QUANTIFICATION OF A STEM SAMPLE WITH VARYING THICKNESS

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Quantitative elemental analysis by scanning transmission electron microscopy combined with energy dispersive X-ray spectroscopy (STEM EDS) is essential for nanoscale materials characterization, yet its accuracy is often limited by specimen thickness and Xray absorption, especially in materials containing both light and heavy elements such as ZnO. Here, we evaluate the influence of specimen thickness on quantitative EDS. A wedge-shaped electron transparent lamella containing a ZnO layer with an expected 50:50 Zn:O composition was prepared by focused ion beam milling. STEM EDS measurements were performed at 200 kV, and an elemental line profile across the ZnO layer was quantified using standardless Cliff-Lorimer, standard-based Cliff-Lorimer, and Zeta-factor methods (available in the ESPRIT software). Cliff-Lorimer approaches exhibit thickness-dependent deviations, with oxygen increasingly underestimated in thicker regions. In contrast, only the Zeta-factor method yields a constant Zn:O ratio matching the expected stoichiometry. Based on these results we discuss under which conditions the Zeta-factor method can enable reliable, thickness-independent quantitative EDS.

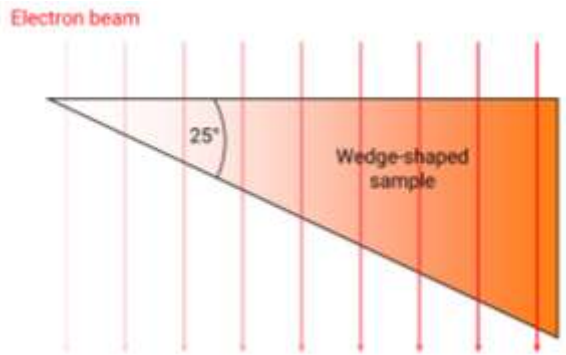

Fig. 1: Side-view diagram of the wedge-shaped sample. During the EDS analysis, the electron beam probes regions of increasing thickness.

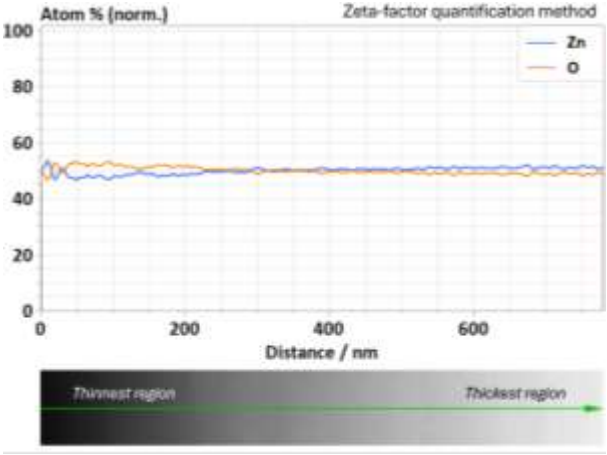

Fig. 2: Atomic concentration along a line profile acquired over a $Zn_{0.5}O_{0.5}$ electron-transparent sample of increasing thickness using the Zeta-factor quantification methods.
Sample and data courtesy: X. Jin, *KIT*

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The TOMO Project – Integrating a Fully Functional Atom Probe in an Aberration Corrected TEM

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In the present contribution, we want to introduce the TOMO microscope which is based on a combination of two well-known but fundamentally different materials analysis techniques in one device: a state-of-the-art atom probe integrated into a high-performance TEM [1-3]. The TOMO instrument represents a novel approach towards atomic-precision imaging and analysis which has not previously been realized. The first important advantage results from the essential complementarity of the techniques, which can be applied to the same local volumes in a consecutive manner. In a correlative approach, local elemental composition at a defect or any other microstructural feature in a given matrix phase can most sensitively be analysed with the atom probe technique, while the atomistic structure and the local bonding situation in a complimentary way can be obtained by HRTEM/STEM and EELS. We will present the design and novel features of the instrument as well as the first results of combined APT/HRSTEM experiments.

We selected three engineering materials for the test experiments: a precipitation-hardened Fe-Cr ferritic steel [4], a Ti-base alloy with grain boundary boron segregation [5] and a BaZrCeYO3 proton-conducting ceramics. With TEM we are able to track the evolution of the specimen shape under APT analyses at near-atomic resolution, which opens up the way to substantially improve the accuracy of 3D reconstructions. The UHV conditions enabled to keep the specimen surface clean for many hours or under electron bean irradiation, eliminating contamination artifacts when combining sequential APT reconstructions. HRTEM helped to reveal some high-field effects such as bending of a grain boundary in the vicinity of the specimen apex. The APT performance in TOMO (mass resolution, signal-to-noise, field of view) was demonstrated to be at the state-of-art level compatible to standalone instruments.

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SIMULATING IMAGES IN TEM: A COMPARISON OF INELASTIC SCATTERING MODELS

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In transmission electron microscope (TEM) imaging, the electrons undergo the effects of inelastic scattering due to phonon excitations. Effects of inelastic scattering cause a gradual decrease in the intensity of the elastic scattering component (elastic channel) of the electron beam. The inelastic scattering on lattice vibrations, also known as thermal diffuse scattering (TDS), plays a crucial role in high-resolution transmission electron microscopy and electron diffraction. The electrons that are inelastically scattered to high scattering angles make up a significant portion of the intensity signal in the dark field. This fact is utilized in high-angle annular dark-field (HAADF) imaging [1,2]. To account for the effects of inelastic scattering, absorptive effects must be incorporated into the simulation of electron propagation through the specimen. Thus, a good model for inelastic scattering is needed. TDS shows up as a diffuse background in diffraction patterns and in simulations, TDS background may differ in shape, intensity, and characteristic features (such as Kikuchi lines) depending on the model used. Various models, which take into account the absorptive effects, exist. We investigate and compare the widely used complex absorptive potentials model to the more elaborate frozen phonon model coming from correlated atomic motion and the Einstein model of atomic motion [3-6]. The complex absorptive potentials model views inelastic scattering as the excitation of the crystal and uses many-body quantum mechanics to describe the absorption [1]. The frozen phonon model is a semi-classical approximative model that represents electron propagation through a static lattice. In the frozen phonon model, the static lattice configurations, so-called snapshots, are obtained via molecular dynamics simulation (in LAMMPS software) with the addition of an interatomic potential, or, in the case of the Einstein model we add random atomic displacements according to known Debye-Waller factors. In this work we compare the different models of TDS via simulating diffraction patterns for diamond and strontium titanate (STO) crystal. For all models, we performed extensive multislice calculations (in Dr. Probe software [7]) for a 300 keV electron beam, which trace the evolution of traversing electron wave function through the crystals, yielding diffraction patterns. The corresponding diffraction patterns are further analysed and compared, as they contain the information about scattering and absorption. We will present the simulation results and discuss non-negligible differences between the models of frozen phonon and complex absorptive model. We will analyse the effects and possible causes of the discrepancies between the simulations acquired by using the different models.

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Geometric Constraints on Quantum Measurement Revealed by Spatially Resolved EELS

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For most of the 20th century, the large size of electron probes restricted our view of nanoscale physical science to electron scattering measurements of energy and momentum. Thus, clusters of nanoparticles showed strong surface plasmons, but very little bulk behavior, suggesting that small structures are dominated by surface/bulk ratio considerations.[1] When nm probes became available, spatially resolved EELS produced local, probe-specimen scattering, rather than momentum resolved averages over many particle volumes. [2] These new results contributed to an exciting period of EELS equipment development aimed at high spatial and energy resolution that continues today.[3]

Theoretical work began with plane waves, to predict energy loss spectra as a function of transferred momentum. Energy transfer was assumed to be *stochastic*, carrying random phase information after scattering. In 1976, Rose proposed a Mixed Dynamical Form Factor to describe simultaneous scattering of waves having well known phases to explore complex shapes of surface plasmons.[4] Nearly 20 years later, in 1993, I used electron probe channeling to cleanly separate plasmon from inter-band scattering in diamond, based on the even or odd lateral parity of the scattered electron wavefunction.[5]

After the success of sub-Ångstrom imaging using aberration correction at the end of the 20th century, observation of individual particle motion under a nanoscale electron beam became obvious, but still difficult to understand.[6] Generally an attractive dielectric response charge would dominate the force between a passing keV electron and a metal particle. Yet for very close approaches, nanoparticles were forced away from the electron beam. Using *time-dependent* calculations based on electromagnetic forces, we found that repulsive magnetic forces overcame dielectric forces at small distances.[7]

These findings of significant dependence on space and time, as well as their *Duals*, momentum and energy, suggest that EELS presents unique capabilities to measure quantum systems that simultaneously display *Dual Behavior*, allowing simultaneous measurements of Dual variables, even near Uncertainty Principle limits.[8] When Dual behavior exists, the geometric space-time algebra of Hestenes can be used to simplify calculations by describing electromagnetic response within a single wavefunction, based on a four dimensional, space-time energy density, and subject to operators constructed to respect well known relationships among electric and magnetic fields.[9] In addition, this kind of treatment couples with ongoing work seeking to unify quantum gravity and electromagnetic behavior, through the AdS-CFT correspondence, a recent conjecture that relates electromagnetic Conformal Field Theory to quantum gravity using String Theory in the Anti-de Sitter geometry that describes space-time near a black hole.[10]

There are experimental results that support this discussion. To illustrate this, I will show a 1973 momentum-energy resolved EELS experiment from Vincent and Silcox [11] that can be Fourier analyzed and transferred to a space-time Penrose Diagram, showing a strong resemblance to entropy information exchange through an event horizon of a Black Hole, described recently by Penington and co-workers.[8]

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TIME RESOLUTION IN TACAW-COMPUTED EELS

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Time-resolved pump-probe experiments offer unique ways for studying ultrafast processes. However, tools for simulating phonon dynamics in electron diffraction patterns at sub-picosecond scales are scarce. In [1], we introduced the frozen trajectory excitation (FTE) method, which enables altering a molecular dynamics trajectory as if it were constantly excited with thermal overpopulation of phonons in a narrow region in the (q, ω)-space. Inspired by the experiment of Tauchert et al. [2], we applied it to fcc Ni. Combined with a modification of the frozen phonon multislice framework, FTE allowed us to plot time-resolved thermal diffuse scattering (TDS) and observe the evolution of a point-like excitation of the TA mode at a sub-picosecond timescale (Fig. 1).
Presented intensities show an excitation appearing at the double momentum transfer (double-q) that can be connected to multi- or multiple phonon scattering, or an ongoing energy transfer. In Fig. 2, we present a higher time-resolution TDS.
To gain more insight into this phenomenon, we pursue a modification of the TACAW method [3] that would introduce the time resolution into it, allowing us to obtain both (q, ω)- and sub-picosecond-time-resolved picture.

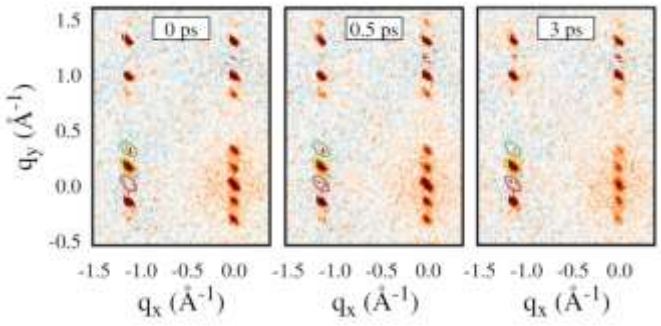

Fig. 1: Relative intensity in TDS at specific time intervals after the point-like excitation [1]. Ellipses (and colors) present the integration area for data in Fig. 2.

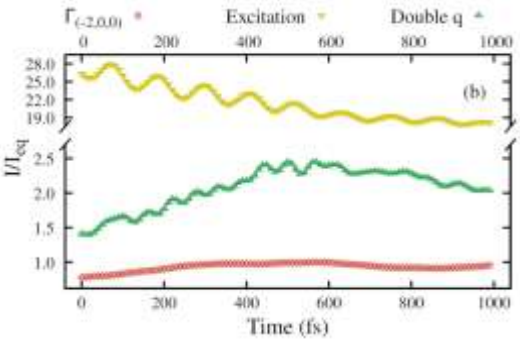

Figure 2: TDS intensity integrated over elliptical regions presented with corresponding colors in Fig. 1 [1].

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Phonon modes decomposition in SiC

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Transmission electron microscopy (TEM) has become a vital tool for probing ultrafast lattice dynamics, thanks to several technological advances. Innovations such as aberration correction, electron beam monochromation for resolving vibrational modes, direct electron detectors, and the integration of ultrafast laser pulses with fast cameras have enabled atomic-scale spatial and temporal resolution. As a result, studies of ultrafast phonon dynamics using electron energy-loss spectroscopy (EELS) are now feasible. Time-resolved pump-probe experiments open unique opportunities to investigate these rapid processes[1,2].

This year, we provided a tool for computationally analysing these experiments by employing the frozen-trajectory excitation (FTE) theoretical framework introduced in [3], which builds upon the reciprocal-space decomposition scheme of the frequency-resolved frozen-phonon multislice (FRFPMS) method [4], [5]. Our goal in this work is to demonstrate the further capabilities of this combined framework to provide valuable insights into mode contributions to diffraction patterns obtained during ultrafast dynamics experiments.

Specifically, we applied the FTE method to analyze various modes in the final EELS diffraction patterns of SiC. Our study examined SiC under both equilibrium conditions and during relaxation following artificially induced excitation, with both states simulated via molecular dynamics. We then decomposed the resulting modes using the FTE framework and performed multislice calculations on the generated snapshots, producing mode- and energy-resolved diffraction patterns.

Acknowledgements
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FFneT project: A deep learning model for detecting frequencies in FFT spectra

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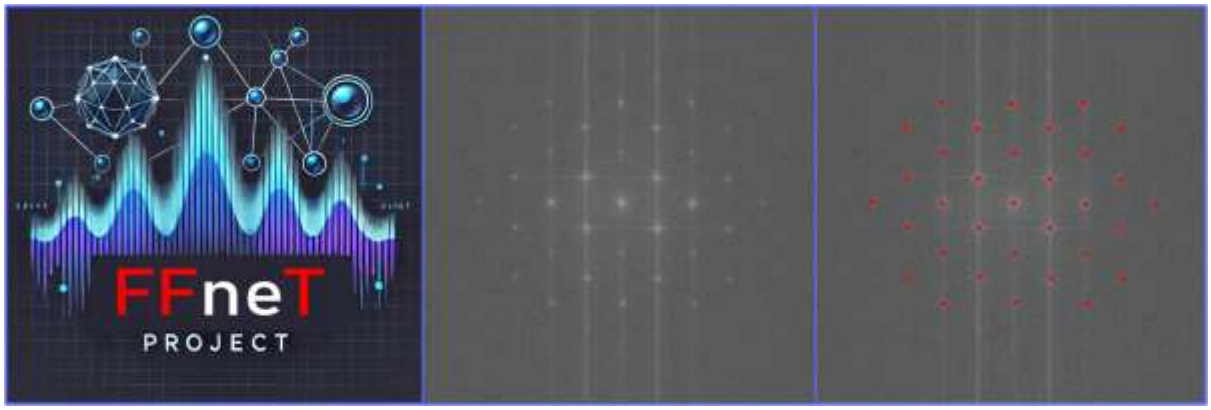
Fast Fourier Transforms (FFTs) are fundamental tools in the analysis of crystalline structures through electron microscopy, providing key insights into lattice periodicities, orientations, and defects. Despite their widespread use, the process of identifying and indexing diffraction peaks within FFTs remains a manual and expertise-dependent task, prone to variability and time constraints. In this work, we introduce **FFneT**, a comprehensive framework designed to automate FFT peak detection and streamline the indexing process using deep learning.

FFneT integrates three core components: (i) the construction of a curated and expandable database of FFTs indexed by crystal orientation and structure type; (ii) the development of a graphical user interface (GUI) to facilitate efficient FFT visualization, annotation, and validation; and (iii) the implementation of a convolutional neural network based on the U-Net architecture, trained to robustly detect diffraction peaks across a wide range of conditions, including varying noise levels and symmetries.

Our preliminary results show that the trained model achieves high accuracy in detecting relevant features in both simulated and experimental FFT data. This framework offers a scalable solution for high-throughput analysis and lays the groundwork for future developments in automated crystallographic characterization. FFneT aims to democratize advanced electron microscopy analysis, enabling both expert and non-expert users to access fast, reliable, and reproducible structural information.



Unified Direct Phase Retrieval Framework and Streaming Parallax Imaging for Efficient Diffractive Imaging

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Direct ptychography enables non-iterative phase retrieval of the electron wave transmitted through a specimen by exploiting interference between the scattered exit wave and a converged probe with known aberrations. Under the weak phase object approximation (WPOA), this framework provides robust information transfer for a range of contrast mechanisms, including single-sideband (SSB), optimum bright-field (OBF), Wigner distribution deconvolution (WDD), parallax imaging, and center-of-mass methods. A key limitation, however, is that spatial resolution is typically bounded by the scan step size, imposing strict sampling requirements that conflict with dose efficiency and acquisition speed.

Here, we present a unified direct ptychography framework in which parallax imaging arises naturally as a quadratic approximation to the phase-compensated SSB reconstruction kernel (Figure 1). This establishes a formal equivalence between parallax and direct ptychography and provides a principled route to scan upsampling within direct phase-retrieval methods [1]. The framework clarifies the respective regimes of applicability, showing that direct ptychography recovers missing contrast transfer at high electron fluence, while parallax offers a robust and dose-efficient alternative for weakly scattering or dose-sensitive specimens.

Building on this formalism, we introduce a fast, streaming implementation of parallax imaging that enables live, upsampled reconstructions during data acquisition (Figure 2). The approach is compatible with modern high-throughput detectors and provides real-time experimental feedback, lowering the barrier for deploying direct phase-retrieval techniques in routine workflows. Finally, we briefly discuss how the assumptions underlying the WPOA and conventional forward models break down at lower accelerating voltages, motivating higher-order multislice algorithms and outlining a path toward extending direct phase-retrieval concepts to emerging low-energy 4D-STEM-in-SEM modalities.

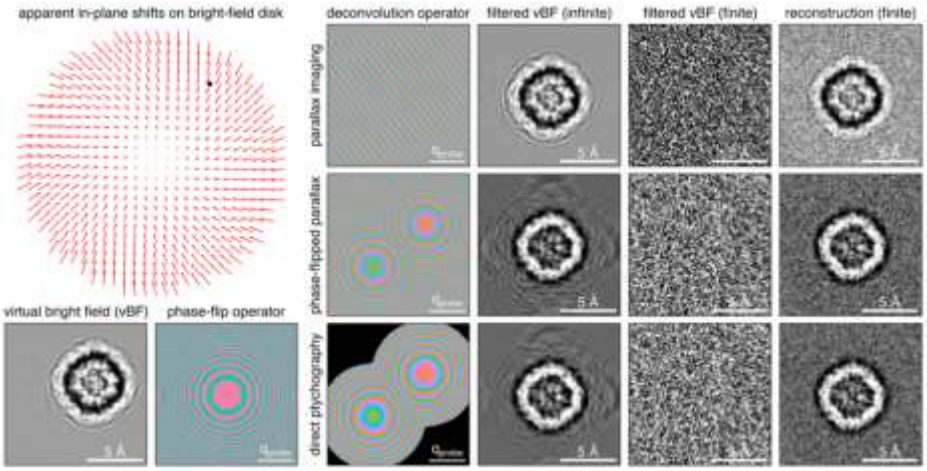

Figure 1: phase-flipped parallax imaging as a quadratic approximation to phase-compensated single-sideband ptychography.

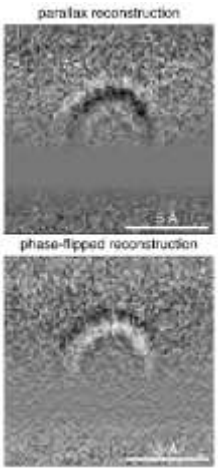

Figure 2: streaming parallax imaging.

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Locally time-resolved scanning transmission electron microscopy (LTR-STEM)

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Four-dimensional scanning transmission electron microscopy (4D-STEM) enables mapping of structural information by recording a diffraction pattern at each probe position. However, materials are not static under electron irradiation. Beam exposure can induce structural degradation, amorphization, or crystallization, i.e., either detrimental or intentional beam-driven phase transformations. In conventional 4D-STEM acquisition, such changes are temporally integrated within each scan position, obscuring the evolution of diffraction intensities and masking transient or dose-dependent behavior. Capturing these dynamics while maintaining signal quality remains a central challenge. Here, we present locally time-resolved STEM (LTR-STEM), an acquisition strategy that extends 4D-STEM into five dimensions by recording rapid diffraction stacks at each scan position. By resolving the temporal evolution of diffraction intensities locally, LTR-STEM enables the separation of signal and damage effects, while preserving spatial resolution. We demonstrate three applications. First, sparsity-based machine learning applied to LTR-STEM diffraction stacks enables denoising prior to summation, significantly improving signal-to-noise ratio in reconstructed 4D-STEM datasets and revealing subtle features such as bending contours in disk-shift maps. Second, analysis of the temporal decay of diffracted intensities within each stack enables direct measurement of the average critical dose of beam-sensitive materials. Third, the kinematics of crystal formation can be quantified by tracking the emergence, growth, and redistribution of Bragg reflections under stationary-beam excitation. By adding a controlled temporal dimension to 4D-STEM, LTR-STEM provides a framework for dose management, denoising, and real-time studies of beam-induced transformations, opening new possibilities for the study of dynamic and beam-sensitive materials.

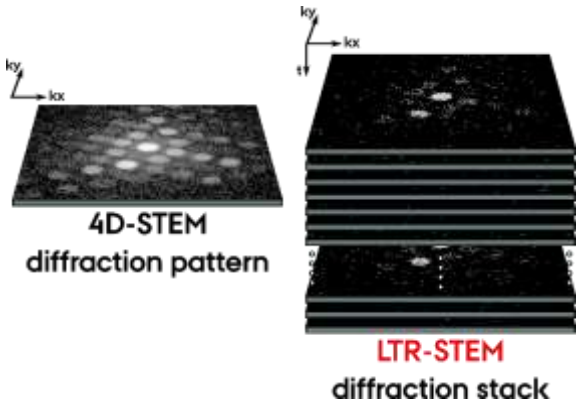

Fig. 1: Concept of LTR-STEM: recording a diffraction stack rather than a single pattern at each scan position.

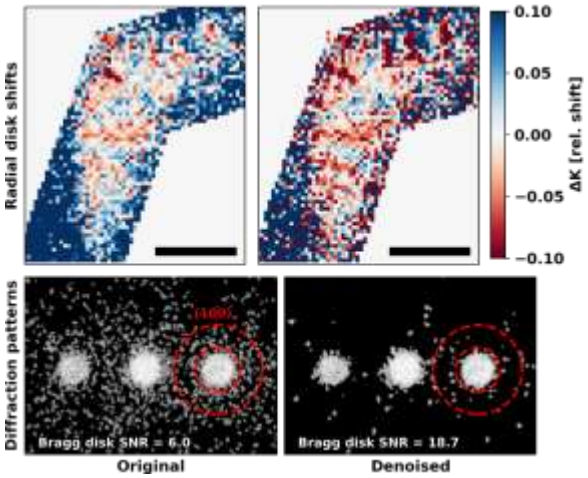

Fig. 2: Machine learning denoising of sparse LTR-STEM diffraction stacks reveals previously obscured bending contours.

BAYESIAN OPTIMIZATION BOOSTED QUANTITATIVE HIGH RESOLUTION TRANSMISSION ELECTRON MICROSCOPY

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Quantitative high-resolution transmission electron microscopy (HRTEM) enables atomic-scale structural determination, but reliable extraction of structural parameters requires iterative image simulations involving a high-dimensional parameter space [1]. Conventional user-guided multi-step refinement is time-consuming and limits quantitative analysis to small areas and expert users.

In this poster, we implement a Bayesian optimization (BO) framework to automate model-based HRTEM quantification. The approach combines trust-region BO with Gaussian process surrogate modeling and a continuous relaxation strategy to efficiently handle mixed continuous–discrete parameters under physical constraints. Imaging-related parameters (e.g., residual aberrations of the imaging lens system, image spread) and structural parameters (atomic positions, occupancies, column atom numbers) are optimized in a stepwise workflow, enabling robust exploration of high-dimensional parameter spaces.

Using a $BaTiO_3$ single crystal that contains heavy, medium and light elements as a model system, we demonstrate that the three-dimensional atomic structure can be reconstructed from a single HRTEM image via parallel region-of-interest matching and integrated model stitching. The BO-boosted workflow achieves stable convergence within minutes, corresponding to a three- to four-order-of-magnitude speedup compared to conventional user-supervised refinement. The method further reveals thickness-dependent suppression of Ti–O displacement in ultrathin regions, consistent with depolarization-driven reduction of ferroelectric distortion.

The proposed framework thus enables fast and automated quantitative HRTEM analysis over extended fields of view and advances structural investigation into the time domain.

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