MERLIN T4: PUSHING THE BOUNDARIES OF STEM/TEM WITH THE NEW TIMEPIX4 ASIC

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Merlin T4 from Quantum Detectors, based on the Timepix4 ASIC developed by the Medipix collaboration at CERN [1], is a next-generation hybrid pixel counting detector for transmission electron microscopy (TEM) that integrates and extends the capabilities of earlier ASIC generations within a single platform. It supports data-driven and frame-based operation. In data-driven mode, individual electron events are recorded with position (X, Y), time of arrival (ToA), and deposited energy (ToT), supporting beam currents up to 200 pA with 196 ps timing precision, while frame mode reaches up to 40k fps with 8-bit dynamic range across the full 512 x 448 pixel array.

This poster highlights the practical advantages of Merlin T4 for TEM applications. Data-driven acquisition enables fast 4D-STEM, correlative, diffraction, EELS, and dynamic TEM microscopy, while frame-based operation accommodates higher currents for nanobeam diffraction and dynamic TEM imaging. Sub-nanosecond timestamping combined with energy measurement further enhances detector performance and enables data volume reduction through post-processing. An example of imaging improvement is demonstrated for a single diffraction pattern in Fig. 1.

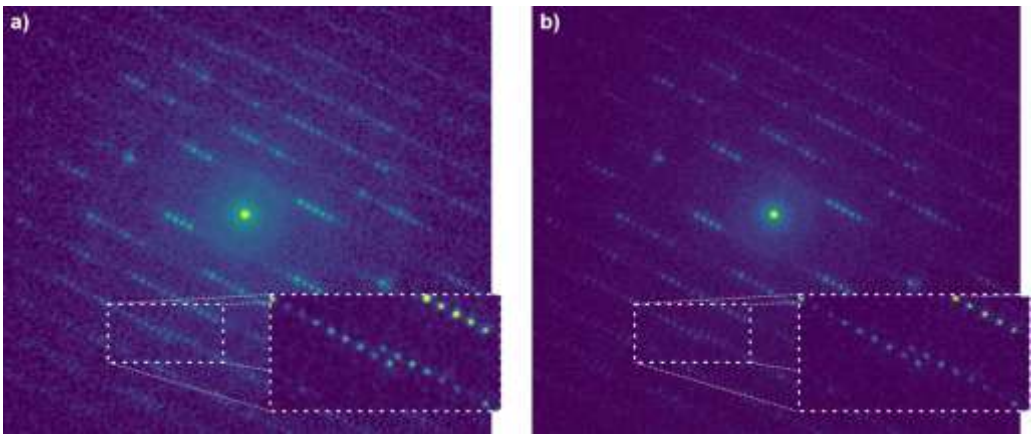

Fig. 1: Merlin T4 diffraction data improvement through post-processing: (a) raw frame; (b) reconstruction using local detector-response analysis and clustering. Main patterns are shown in logarithmic contrast; inset details are shown in linear contrast. Data were acquired on a JEOL cryoARM microscope (Crewe) at the Rosalind Franklin Institute with 200 kV beam energy; frames correspond to a 0.782 ms snapshot during continuous tilt of a biotin sample. [2]

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[2] Acknowledgements: Marcus Gallagher-Jones, Zhiyuan Ding, Angus Kirkland, Rosalind Franklin Institute

Precession-enhanced Electric Field and Pair Distribution Function mapping in the Transmission Electron Microscope

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The use of a precessing electron beam in 4DSTEM for improving the quality of diffraction patterns is well known in literature. The same methodology can also be applied for tackling other materials analysis problems such as the measurement of local fields in the sample [1] and the characterization of amorphous materials [2].

In this poster, we will demonstrate the advantages of using precession for electric field measurements, and describe how we aim to extend this application to the mapping of local magnetic fields. Additionally, we will show results on the automatic analysis of short-range order in amorphous materials from 4DSTEM maps using the electron Pair Distribution Function analysis, and present our roadmap on extending this capabilities towards amorphous phase mixtures and strained amorphous materials.

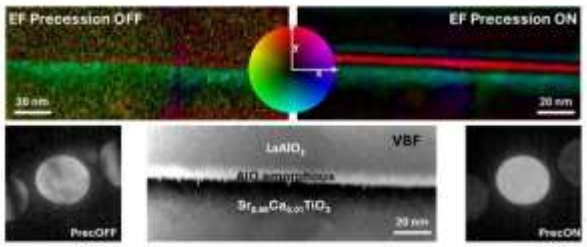

Fig. 1: Example of the benefits of precession in an e-field mapping experiment.

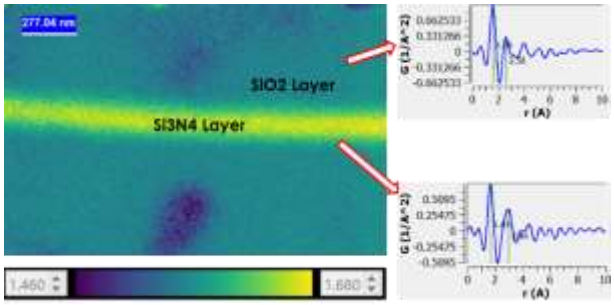

Fig. 2: Determination of short range order in a semiconductor device cross-section.

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Streamlined Software for 4D STEM Experiments and Real-Time Virtual Detector Calculation

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With its broad range of applications, 4D STEM is increasingly used as a standard technique. To minimize overhead and simplify usage, we developed EMplified Scan, a software package that supports 4D STEM acquisition with TVIPS TemCam-XF cameras and DECTRIS hybrid detectors, such as QUADRO and the ultra-fast ARINA detector. Synchronization of scanning and image acquisition is handled by the TVIPS Universal Scan Generator. The datasets are stored in lossless compressed HDF5 format with complete metadata for seamless postprocessing.

EMplified Scan enables real-time computation of virtual detectors, allowing multiple custom detectors to be displayed alongside standard STEM detectors during continuous acquisition. It also integrates essential microscope control functions, including automatic beam blanking and detector insertion/retraction.

Camera systems from TVIPS and from DECTRIS can be integrated into EMplified Scan, making it a flexible solution for upgrading JEOL or TFS microscopes with 4D STEM capability. Performance examples are:

- DECTRIS ARINA: 1024 × 1024 scan with 2× binned pixels (96 × 96 pixels) in <10 s.

- TVIPS TemCam-XF416ES: 100 x 100 scan at a camera format of 1024 x 1024 pixels in <1 min. It offers a large resolution and field of view of up to 4k x 4k pixels with a pixel size of 15.5 µm.

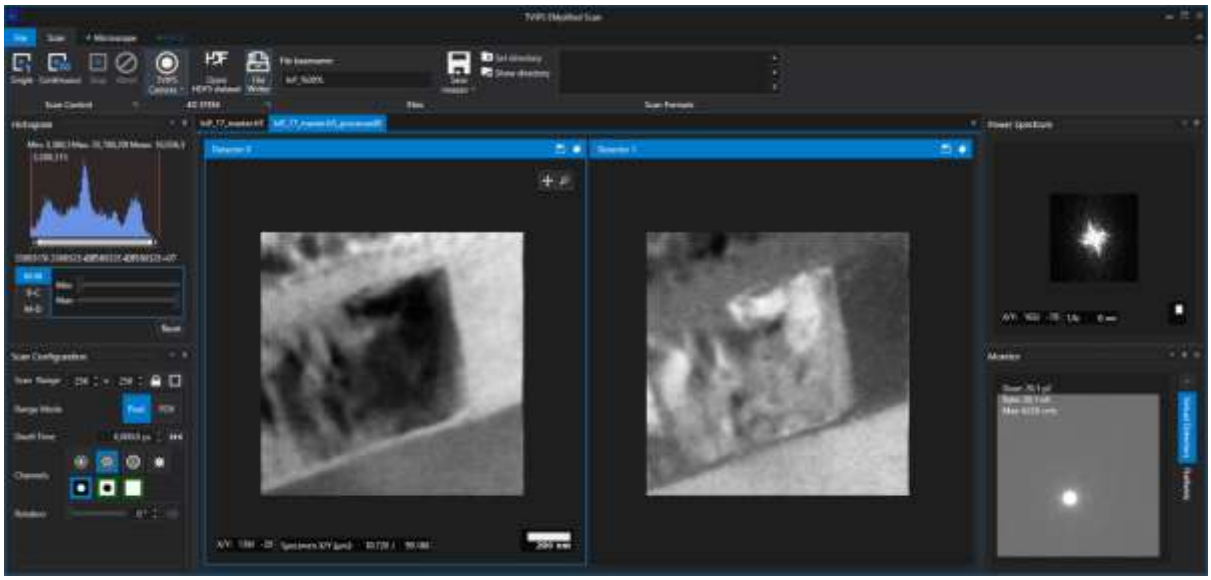

Fig. 1: Screenshot of EMplified Scan showing virtual dark and bright field detector images of a cross section of sputtered InP. The monitor image (right lower corner) shows the live diffraction pattern on a TemCam-XF416.

INELASTIC ELECTRON-LIGHT INTERACTION PROBED BY HOLOGRAPHIC SCANNING TRANSMISSION ELECTRON MICROSCOPY

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Ultrafast transmission electron microscopy (UTEM) has been an established method for investigating stimulated inelastic scattering between free electrons and optical near-fields for several years. The optical near-field imprints a sinusoidal phase modulation on the electron wavefunction, which results in a comb of sidebands in the electron kinetic energy distribution. In recent years, there have been experimental developments to reveal the near-field phase by employing defocus phase-contrast microscopy [1,2] or sequential interactions as a complementary approach [3]. While offering high resolution, sensitivity, and robustness, these techniques rely on particularly high beam coherence, specialized sample holders and multi-parameter scanning, which complicates their experimental implementation. Therefore, holographic approaches at somewhat reduced coherence requirements, simplified geometry, and enhanced flexibility in tailoring the interaction are desirable.

In this contribution, we combine scanning transmission electron microscopy with spatially separated coherent electron probes [4] and parallel electron-light interactions. Multiple STEM foci are prepared by employing an amplitude diffraction grating in the electron microscope condenser system. Relative phase information is retrieved from the interference pattern recorded in the far field. In general, the visibility of the hologram reflects the coherence between the interfering beams that is typically reduced by inelastic processes. However, in the context of inelastic, coherent manipulation of electron states by optical near-fields, the visibility encodes distinguishability, which can be controlled by the interaction strength. By adding an electron spectrometer, we can observe the interference pattern as a function of energy. This enables simultaneous access to the energy of the electrons and the phase imprinted during the inelastic interaction. Furthermore, superimposing multiple parallel interactions grants access to spectral distributions of the electrons that are not achievable with a single interaction. Our results reveal unconventional electron states, whose emergence and properties are governed by the interplay of interaction strength and relative phase differences. Beyond the preparation of tailored quantum states, deep insights into quantum coherence and correlation effects are provided.

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Characterisation of antiferromagnetic $NiPS_3$ using TEM and ptychography simulations

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Magnetic materials have been employed for a wide range of applications in electronic technology, such as magnetoresistive random access memory, spintronic devices, magnetic sensors, and quantum information technologies. Two-dimensional (2D) magnetic materials have further attracted extensive attention due to their applications in devices with smaller sizes and lower power consumption, which is realised by their unique physical properties at the atomic scale. Different 2D materials can also be stacked together to form heterostructures, which can exhibit new physical properties different from those of the original materials. In addition, when external stimuli such as electric fields or strain are applied, the properties of these materials can change significantly. Since many of their properties manifest at extremely small length scales, transmission electron microscopy (TEM) can be used to study their microscopic structure and properties.

The microstructure and magnetic properties of ferromagnetic 2D materials, such as the CrX_3 family, the $Cr_2Ge_2Te_6$ family, the Fe–Ge–Te family, and magnetic transition metal dichalcogenides (TMDs), have been successfully studied using the TEM due to their relatively large magnetic domains. Using Lorentz TEM, magnetic features such as magnetic domains or skyrmions can be observed near the Curie temperature. Antiferromagnetic materials, such as the MPX_3 family (M = transition metals including Mn, Fe, Ni, and X = trichalcogenides including S and Se), are also widely studied magnetic materials. In this structure, the metal ions form a honeycomb lattice, and the $[P_2X_6]^{4-}$ units are located at the centre of the hexagon formed by the metal ions. Among the MPX_3 family, $NiPS_3$ has a relatively high Néel temperature of about 155 K. Previous theoretical calculations indicate that the in-plane magnetic moments of $NiPS_3$ exhibit a zigzag antiferromagnetic ordering, while the interlayer coupling is ferromagnetic. Because antiferromagnetic materials do not exhibit net macroscopic magnetisation, it is necessary to study antiferromagnetic materials using TEM at atomic resolution. However, there are still limitations in studying their magnetic structures using different TEM techniques including electron diffraction, ptychography, and differential phase contrast (DPC), which also leads to significant debates and discussions in the field. [1][2][3]

In this work, image and diffraction simulations are used to investigate the crystal structure of the antiferromagnetic material $NiPS_3$, and ptychography simulations are performed to optimise parameters for ptychography experiments. The atomic model of $NiPS_3$ was first created using the abTEM software. Scanning TEM (STEM) and diffraction simulations were carried out to identify the changes in STEM images and diffraction depending on the thickness of the 2D material. Ptychography simulations were also performed in order to select suitable reconstruction methods and to optimise parameters for the experiments. In addition, simulations incorporating magnetic potential fields were attempted to explore possible approaches to investigating magnetic information in this material.

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Correlated atomic vibration imaging with sub-ångström resolution

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In transmission electron microscopy, thermal diffuse scattering [1] is an obstacle that limits the achievable resolution of any coherent phase-retrieval technique. It has been shown that electron ptychography can overcome resolution limits arising from aberrations and partial coherence of the illumination, but not those imposed by atomic vibrations [2]. Here, we propose a reconstruction framework for electron ptychography [3] that explicitly accounts for thermal diffuse scattering and opens an entirely new channel of information about the phonon dispersion of a sample without the need for a spectrometer. Our method relies on a combination of the mixed-object formalism [4], in which a sample is treated as an incoherent superposition of states, and Green's tensor analysis [5], which is well established in the molecular dynamics community. In Figure 1, we show a reconstruction from experimental data for hexagonal boron nitride. Using only the atomic masses and the temperature as input, we obtain interatomic correlations, schematically shown by arrows, and average phonon frequencies of 10.8±0.1, 13.6±0.6, 18.0±0.2, and 25.5±1.5 THz for the longitudinal and transverse acoustic and optical phonons, respectively. This ability to spatially resolve correlated atomic motion distinguishes our method and positions it as a complementary tool to vibrational electron energy-loss spectroscopy [6] for exploring atomic dynamics at the finest scale. It has the potential to be instrumental in the development of phononic devices, in the study of phonon-based decoherence in quantum systems, and in other emerging phonon-based applications.

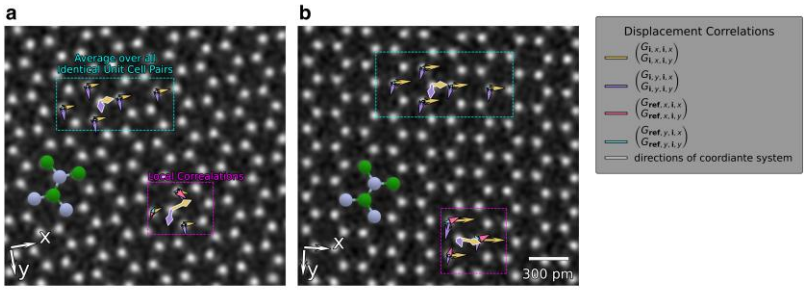

Figure 1. Interatomic correlations recovered from experimental mixed-object ptychographic reconstruction of approximately 15 nm thick twisted hBN bicrystal. a, b, Projected potentials of the two parts of a bicrystal, which are stacked vertically on top of each other, such that every detected electron has passes through both of them. The arrows represent various components of the retrieved Green's tensors. Arrows with white outlines correspond to reference atoms; yellow and purple arrows indicate correlations of atoms with their own displacements along the x and y axes, respectively. Pink and light-blue arrows show correlations of atoms with displacements of a reference atom along the x or y direction. Magenta dashed boxes highlight correlations corresponding to a particular atomic column (and its neighbors), while turquoise boxes show correlations averaged over all identical unit-cell pairs.

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Quantum Nuclear Effects in Temperature-Dependent EELS

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The time autocorrelation of auxiliary wave (TACAW) method has established a framework for modeling angle-resolved electron energy loss spectroscopy (EELS) by deriving scattering intensities from the time autocorrelation of the beam wavefunction [1]. This approach enables efficient computation of scattering intensities while naturally accounting for dynamical diffraction and multiple-scattering effects. In the cryogenic regime, vibrational spectra are dominated by nuclear quantum effects, notably zero-point motion and tunneling. To capture these effects in low-temperature vibrational EELS, we incorporate the thermostatted ring polymer molecular dynamics [2] into the TACAW formalism. Our calculations on silicon reveal that quantum nuclear effects significantly alter the vibrational spectra compared to classical molecular dynamics predictions, indicating that quantum nuclear effects cannot be neglected even in simple systems at low temperatures. This method provides a robust theoretical tool for probing the low-temperature limit of vibrational EELS, offering a necessary benchmark for the quantitative analysis of emerging cryogenic scanning transmission electron microscopy experiments [3].

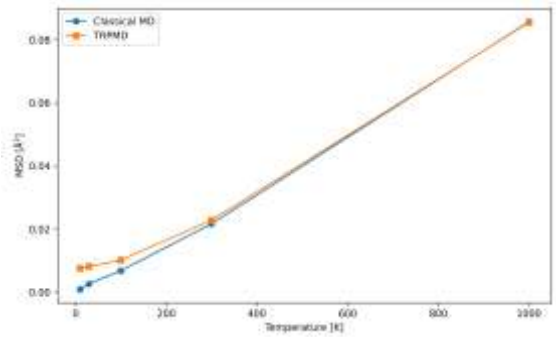

Fig. 1: The mean-square displacement of silicon is evaluated over temperatures from 10 K to 1000 K and compared between classical molecular dynamics and thermostatted ring polymer molecular dynamics.

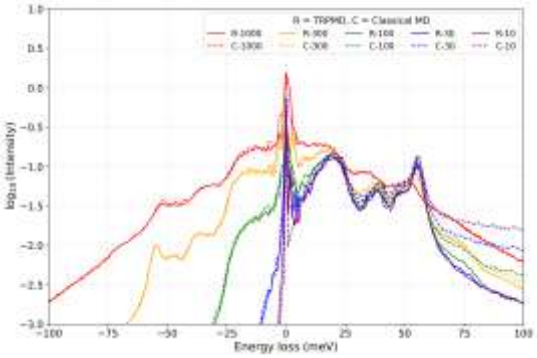

Fig. 2: EELS spectra of silicon at temperatures ranging from 10 K to 1000 K, displayed on a logarithmic intensity scale.

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STEM-EELS: COMPUTATIONAL STUDY OF VIBRATIONAL DYNAMICS OF DEFECTS AT ATOMIC-SCALE

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Last decade's advancements in instrumentation for electron energy-loss spectroscopy (EELS) in scanning transmission electron microscopy (STEM) have enabled unprecedented insights into local vibrational properties with energy resolution below 10 meV while keeping the spatial resolution subatomic [1-4]. We will present how the time-autocorrelation of auxiliary wavefunctions (TACAW) method [5] was used to model energy-resolved STEM-EELS experiments with subatomic resolution performed on a sample of TiO_2 with planar defects. With off-axis detector geometery, we further investigate the measurements and simulations in terms of vibration polarization [6-8].

By utilizing off-axis detector geometries, we selectively capture phonon modes with specific polarization vectors, allowing direct visualization of vibrational characteristics with atomic precision. Our methodology provides an interesting framework for exploring thermal transport mechanisms at the atomic scale. Our workflow leverages machine-learned-interatomic-potential (MLIP) Orb2 [9] to drive molecular dynamics (MD) simulations. This enables faster computation of MD trajectories (with optional GPU acceleration) which are prerequisites for TACAW based simulations of STEM-EELS signal.

Preliminary experimental and theoretical results, which will be shown, reveal complex structure of vibrational modes on a planar defect in a crystal of rutile (TiO_2) and offer direct insight into the complex heat transfer mechanisms at nanoscale.

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ATOMIC-SCALE DOUBLE-SLIT INTERFERENCE REVEALS CORRELATED ATOMIC VIBRATIONS

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Understanding local phonon transport in nanostructured materials requires probing not just static atomic positions but also dynamical properties, specifically inter-atomic vibrational correlations. Recent advances utilizing segmented[1] and pixelated detectors[2], as well as electron energy-loss spectroscopy (EELS)[3], have enabled the detection of local phonon states and subtle signatures of atomic motion. Crucially, 4D-STEM technology now offers the potential to target individual atomic pairs to capture detailed convergent-beam electron diffraction (CBED) patterns necessary for quantitative vibrational analysis. Here, realizing this capability, we demonstrate that crystalline materials can function as atomic-scale double-slit interferometers using aberration-corrected STEM[4].

We positioned a focused electron probe precisely between two adjacent Si atomic columns separated by 1.36 Å (Si[110] dumbbell). In this geometry, the attractive potential of the atomic nuclei acts as a waveguide, effectively creating two coherent point sources at the exit surface. Using a high-speed pixelated detector, we observed distinct interference fringes in the diffraction patterns corresponding to the 1.36 Å separation.

Crucially, these interference fringes persist even at elevated temperatures up to 900 K. Comparison with frozen-phonon simulations reveals that the standard Einstein model, which assumes independent atomic vibration, fails to reproduce the high-angle fringes. Instead, the data is only explained by a model incorporating correlated thermal vibrations. We found that neighboring atoms vibrate preferentially in-phase, preserving the effective slit separation and thus the coherence of the scattered electrons.

Leveraging this mechanism, we quantitatively extracted the directional correlation coefficients from the fringe visibility. This method allows us to visualize local atomic arrangements and encode dynamical bonding information at the single atom-pair level. By recasting the crystal as an interferometer, this approach opens new pathways to probe phonon-mediated phenomena and local stiffness with atomic resolution.

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HIGH-PERFORMANCE C++/CUDA WAVEFRONT PROPAGATION FOR REAL-TIME BEAM SHAPING: A DETERMINISTIC PHYSICS ENGINE FOR ELECTRON MICROSCOPY

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The integration of laser-based beam shaping via Spatial Light Modulators (SLMs) is transforming electron microscopy, enabling dynamic quantum state engineering and advanced aberration correction [1], [2]. However, navigating the high-dimensional parameter space of light-electron interactions requires a predictive Digital Twin capable of real-time, high-fidelity simulation [3]. Traditional wavefront propagation algorithms face a severe computational cliff at high space-bandwidth products; standard direct matrix methods scale at $O(N3)$ and bottleneck real-time instrument control, making interactive optimization humanly impossible. To overcome this, we present a high-performance C++/CUDA framework that serves as a deterministic, ultra-low-latency physics engine for complex light- and electron-optics simulations.

By implementing a separable 2D Zoom Propagator based on the Chirp Z-Transform (CZT), our framework decouples the simulation grid from physical sampling constraints, achieving $O(N2logN)$ algorithmic complexity. We detail a hardware-aware CUDA architecture optimized for NVIDIA Ampere GPUs, featuring a zero-allocation memory pool that eliminates OS-level heap latency during iterative loops. Furthermore, by utilizing padded shared memory for conflict-free tiled transpositions and maximizing arithmetic intensity through kernel fusion, the engine achieves 98% memory bandwidth efficiency (745 GB/s). Benchmarks demonstrate sub-30 ms iteration times even at massive 8K resolutions (an 8192 x 8192 grid) of the holograms.

Crucially, this raw computational velocity and the developed API infrastructure establish the necessary foundation for future autonomous control systems. While current automated tools lack physical grounding, our framework exposes low-latency APIs specifically designed for the future integration of a Multimodal AI Co-Pilot [4], [5]. In this forthcoming architecture, an AI agent will act as a high-level frontend, while the current C++/CUDA physics engine serves as a strict "System 2" safety valve. By validating proposed phase masks in milliseconds ensuring wavefront intensity and sample dose thresholds are met before hardware execution this physics engine bridges high-performance computation with future agentic AI, paving the way for the safe, autonomous operation of next-generation electron microscopes.

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MOMENTUM-RESOLVED EELS FOR ELEMENTAL MAPPING VIA 3D RECONSTRUCTION

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Cryo-electron microscopy provides an increasingly detailed view of the structure and function of macromolecular complexes, but lacks a technique to map species bound within these complexes. Elemental information is accessible in the EM via scanning transmission electron microscopy-electron energy loss spectroscopy (STEM-EELS), but the high dose requirement prohibits its direct application to cryopreserved samples. Recently, we showed that this can be circumvented by accumulating signal through 3D reconstruction of spectral images (SI) of many identical complexes. In that work, we calculated the pose information (position and orientation of a macromolecule) for 3D reconstruction using elastic bright field (EBF) reference images. This information was then used for 3D reconstruction of densities for each energy loss in the correlated EELS-SI (Fig. 1) [1]. The success of this approach was limited by the inefficient contrast generation in EBF images, which could be improved by implementing phase contrast image generation in parallel with spectral data acquisition. One mode of phase contrast imaging that is available in focused-probe STEM mode is integrated center-of-mass (iCOM). In this mode, the 2D center-of-mass (COM) shift in the bright-field region of a convergent beam electron diffraction (CBED) pattern is measured at each scan position, and this vector field is integrated to give an image that is linear in the project potential of the sample [2]. The COM vector is normally measured either on a pixelated detector, or using a segmented STEM detector. Recently, momentum- and energy-resolved EELS (q-EELS) data was used to generate an iCOM image, achieving atomic resolution images [3]. In this scheme, momentum information is retained in the non-dispersive direction and provides one component of the COM vector [3]. The perpendicular component can be recovered by performing a second scan over the same area with a 90° rotation of diffraction space (Fig. 2) [3]. Sample drift between scans is corrected. Here, we demonstrate the application of this scheme on a biological sample.

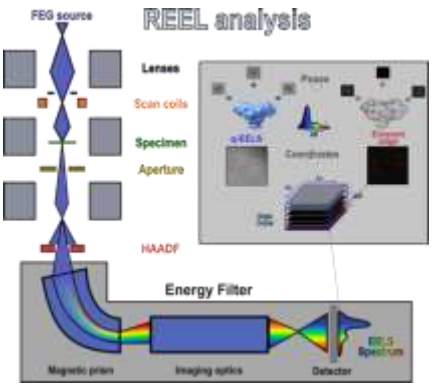

Fig. 1: REEL analysis data processing.

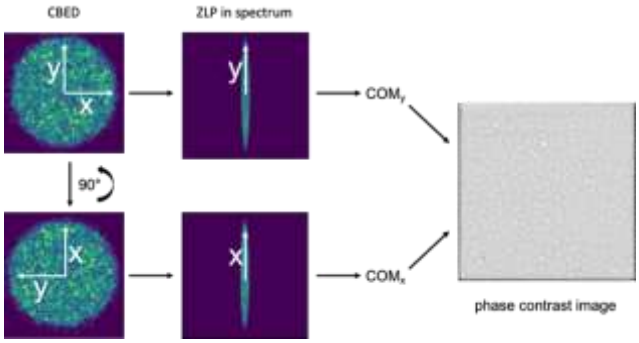

Fig. 2: Phase contrast imaging by q-EELS.

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[3] B. Haas and C. T. Koch, Microsc. and Microanal., vol. 28, no. S1, pp. 406–408, (2022)