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Contrast Optimization Aided by Machine Learning Applied to Virtual 4D-STEM Images

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Scanning Transmission Electron Microscopy (STEM) has revolutionized imaging due to its high spatial resolution and easy interpretation due to varied contrast mechanisms, such as atomic number (Z) contrast at high-angle scattering and phase contrast from the bright-field disk. The enhanced flexibility in terms of scattering range detection in comparison with STEM is one of the reasons that led to the increased interest in 4D-STEM [1]. Supported by the recent evolution of pixelated detectors, 4D-STEM currently allows for the recording of the complete electron scattering range at speeds commensurate with traditional STEM experiments [2]. With the possibility of flexible reconstruction of virtual STEM images with arbitrary detector shapes, contrast optimization for sample regions with different scattering cross-sections is envisioned. This study delves into the optimization of contrast in virtual 4D-STEM images, employing both user-guided and machine-learning (ML) optimization approaches.

Reference samples from semiconductor devices and supported catalysts were measured with fast 4D-STEM under experimental conditions mirroring standard STEM imaging practices, with 1024x1024 scan positions and 10 us dwell time. The resultant datasets comprised 106 diffraction patterns with 96x96 pixels each, presenting a great challenge for manual contrast optimization due to the vast data volumes and nuanced contrast differences within the areas of the specimens. Figure 1 shows manual contrast optimization applied to virtual 4D-STEM images, serving as a foundational comparison point for our machine learning (ML)-aided methodology. The left panel reveals a virtual Bright Field (BF) STEM image, with an inset in the upper left corner illustrating a typical example of electron scattering and the application of a virtual mask overlay, highlighting the initial manual approach to contrast enhancement. The center panel demonstrates a virtual STEM image that has been collected utilizing an optimized annular mask, reflecting the outcomes of manual contrast optimization efforts. In the right panel, a line profile from these virtual images is presented, with indications of contrast levels, offering a quantitative perspective on the enhancements achieved through manual methods.

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This figure effectively sets a benchmark for the subsequent introduction of our ML-aided approach, illustrating the initial state of contrast optimization against which the improvements facilitated by automated, ML-driven processes can be measured. By providing a clear depiction of manual optimization efforts, Figure 1 underscores the necessity and impact of transitioning towards more sophisticated, automated methodologies for contrast enhancement in 4D-STEM imaging.

In the current study, we develop an innovative computational framework designed to automate the enhancement of contrast in similar regions within 4D-STEM data. Our methodology integrates the advanced deep learning architecture, ResNet101 [3], for feature extraction, followed by Principal Component Analysis (PCA) for dimensionality reduction, and the application of hierarchical clustering techniques (Figure 2). The utilization of ResNet101, distinguished for its deep residual learning capabilities, is strategically chosen to adeptly capture the nuanced, hierarchical features inherent in 4D-STEM datasets, which are pivotal for identifying similarities across various regions. The initial phase of our analysis involves processing the 4D-STEM diffraction patterns through the ResNet101 model, which has been pre-trained on extensive image datasets. This step is instrumental in extracting comprehensive high-dimensional feature vectors that encapsulate the essential attributes of each pattern. Such a transformation of raw diffraction data into a quantitative form surpasses traditional manual feature identification methods, which are often subjective and labor-intensive, by leveraging automated, objective feature extraction. Following feature extraction, we employ PCA to transform the high-dimensional feature space into a lower-dimensional one, effectively reducing the computational complexity while preserving the variance critical for subsequent analysis. This dimensionality reduction is crucial for enhancing the tractability and interpretability of the dataset, allowing for a focused examination of the significant variances among diffraction patterns. The analysis concludes with hierarchical clustering, an agglomerative method that iteratively merges data points based on their similarity, thereby organically identifying clusters of similar regions without the need for predefining the number of clusters. This method is selected for its adaptability in uncovering the inherent groupings within the data, thereby facilitating an intuitive understanding of similarities across the dataset. The dendrogram generated in this process serves as a pivotal tool for visually determining the grouping of similar regions, thereby informing the selection of clusters for targeted contrast enhancement.

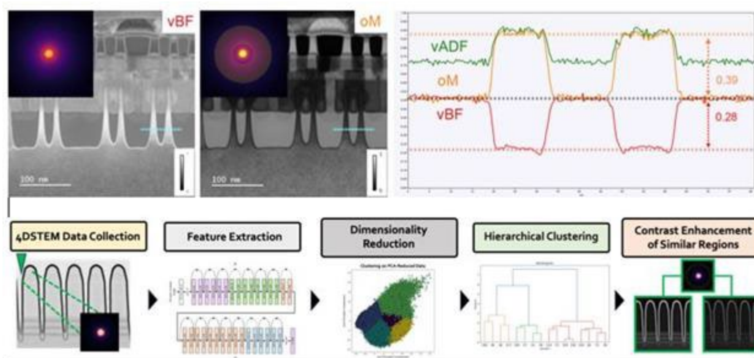
This integrated approach—merging deep learning-based feature extraction, PCA, and hierarchical clustering—presents a robust strategy for automatically enhancing the contrast of similar regions within 4D-STEM data.

By doing so, it significantly advances the automation of contrast enhancement, ensuring more efficient, accurate, and objective analysis of material structures. This methodology helps to streamline the process of identifying and enhancing similar regions within complex materials.[4]

Fig. 1. (left) Virtual BF STEM image, inset (upper left) indicates an example scattering and with the virtual mask overlay. (center) Virtual STEM image collected with an optimized annular mask. (right) Line profile from virtual images with the relative contrast level calculated from normalized intensities,with an An contrast increase from 28% to 39% is observed between images reconstructed from virtual BF and with an optimized annular mask.

Fig 1. B) Workflow applied for the ML-based contrast optimization.

Graphic:



Keywords:

4D STEM, contrast enhancement

Reference:

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