ePattern: an adaptive 4D-STEM Pattern Registration Algorithm to Optimize ACOM Pattern Matching

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The technique known as four-dimensional scanning transmission electron microscopy (4D-STEM)1 has recently emerged as a potent tool for the local characterization of crystalline structures in various materials, including cathode materials for lithium-ion batteries and perovskite materials for photovoltaics.

This 4D-STEM data analysis method based on the ACOM system of NanoMegas (Astar)2,3 uses pattern matching of a scanning nano-diffraction dataset with libraries of diffraction patterns simulated from known structures extracted from CIF files. This method enables to construct crystalline phase and orientation maps to determine crystallinity4,5, microstructures6, structural deformation7, and grain boundaries8 using scanning nano-diffraction with precession mode in a nanometer resolution9,10. However, the utilization of new detectors specifically designed for electron diffraction patterns and other advanced techniques necessitates the continuous adaptation of methodologies to address the challenges associated with crystalline materials.

The goal of the data preparation methods proposed here is to improve the quality of Astar pattern-matching using a dataset of diffraction patterns acquired with a CMOS Oneview camera. The high sensitivity of the CMOS camera and the data filtering developed here modify the diffraction images leading to a compromise between improving image quality and optimizing template-matching results11.

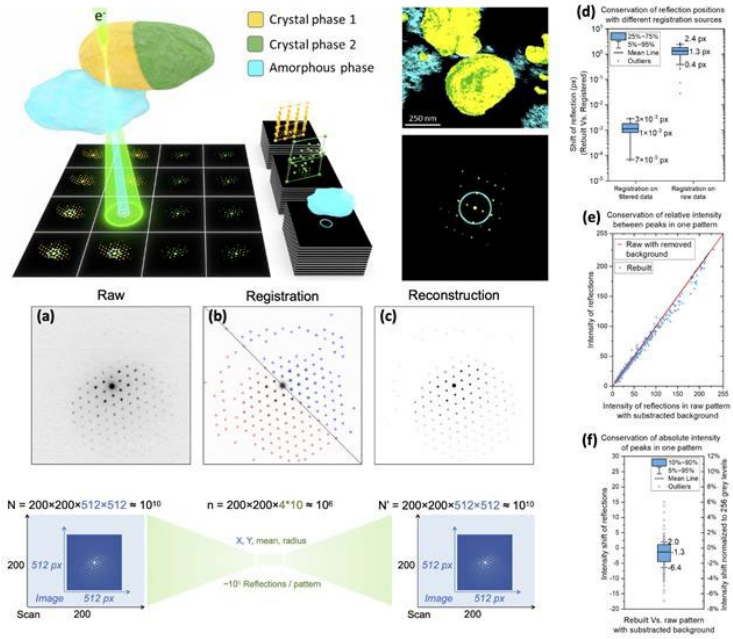
Our strategy employs a data reduction technique that utilizes registration methods to identify electron diffraction spots within patterns. By doing so, we are able to filter and capture the diffraction signal and subsequently reconstruct the patterns. These reconstructed patterns are then inputted into the Astar suite pattern-matching software. This process allows us to record the essential information of each reflection in a dataset, including intensity, size, and position, with a high level of accuracy (sub-pixelar) for the position, typically on the order of 10-3px. Additionally, this technique achieves a significant reduction in data size, typically by a factor of 103. This means that the essential information of the diffraction pattern is stored on a disk with

100 to 1000 times less space required. The adaptative nature of this method not only reduces noise and compresses nanodiffraction scanning data for ACOM and strain mapping analysis but also extends its applicability to other techniques such as 3D electron diffraction (3DED).

To evaluate our approach, we employ dedicated metrics that clearly demonstrate a substantial improvement in phase recognition. Our results indicate that this data preparation method not only enhances the quality of the resulting image but also boosts confidence levels in the analysis of crystal orientation and phase determination outcomes. Furthermore, it helps mitigate the potential impact of user bias that may arise when manipulating parameters during the application of this method.

Firstly, modifications on inside diffraction patterns are estimated through image quality metrics such as peak signal-over-noise (PSNR), structural similarity index measure (SSIM), and root-mean-square error (RMSE). Secondly, the quality of the pattern-matching process on filtered and reconstructed images obtained by the proposed experimental data preparation method is evaluated using index and orientation reliability, as defined in the Astar software. We demonstrate that the experimental data preparation helps to improve the pattern-matching quality result, as it reduces noise overfitting, improves structural similarity index measure, and increases the orientation reliability.

Graphic:



Keywords:

4D-STEM ACOM, ePattern software, diffraction-pattern

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