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Unsupervised Machine Learning-based STEM diffraction pattern denoising for enhanced grain visualization in phase change materials

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Background

Phase change materials (PCM) are an emerging class of materials in which different phases of the same material may have different optical, electric, or magnetic properties and can be used as a phase change memory [1]. Phase-change memory materials, exemplified by (Ag, In)-doped Sb2Te (AIST) in this research, have several advantages, including high-speed read and write operations, non-volatility, and a long lifespan [2]. PCMs are able to switch between amorphous and crystalline phases when subjected to heat or electrical current. However, the full understanding of PCMs depends heavily on accurate characterization, often through techniques such as scanning transmission electron microscopy (STEM).

In the field of materials science and nanotechnology, the analysis of STEM diffraction patterns is crucial for understanding the structural characteristics of materials, especially in the context of PCMs. Accurate interpretation of diffraction patterns is essential for crystallographic analysis, phase identification, and grain visualization during an in-situ switching experiment. However, the analysis of STEM diffraction patterns in PCMs can be challenging due to the presence of noise and weak signals (Fig.1 left).

Methods

In this study, we present a solution to address the challenge of grain visualization in PCMs. We propose an unsupervised machine learning (ML) approach that employs an autoencoder to denoise STEM diffraction patterns. Autoencoders are neural network architectures that have the ability to learn in an unsupervised manner and that are able to represent complex data in a lower-dimensional, noise-reduced form [3]. By applying this technique, we enhance the quality of diffraction patterns, improving the signal-to-noise ratio, which is highly beneficial for further analysis and visualization.

Results

Our results demonstrate a significant enhancement in the clustering and visualization [4] of crystalline grains within STEM diffraction patterns of phase change materials. By reducing noise and enhancing signal clarity, the unsupervised ML-based denoising technique allows for more precise discrimination between different crystallographic orientations and refines the identification of grain boundaries.

Furthermore, we employed clustering based on the non-zero order peak position. Nnotably, this approach yielded significantly improved results for the denoised data (Fig. 2).

Additionally, the proposed denoising enhances pattern-matching quality in commercial orientation mapping software (ACOM ASTAR), indicated by higher average index values and more visible structure in index maps, as illustrated in Fig. 3), facilitating precise analysis of crystallographic orientations and grain boundaries.

Conclusion
The proposed approach paves the way for a deeper understanding of phase change behavior, aiding in designing and optimizing PCMs for various applications, from thermal energy storage to non-volatile memory technology.

As an unsupervised method, it does not require the laborious production of specific training data and, therefore, can serve as a universal tool for STEM diffraction pattern denoising and signal enhancement. Last but not least, the proposed denoising technique is not limited to PCMs; therefore, our work can be understood as a general strategy for enhancing diffraction patterns.

Graphic:

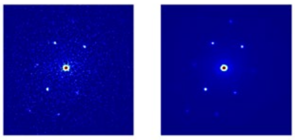

Fig. 1: The diffraction pattern before (left) and after (right) the denoising

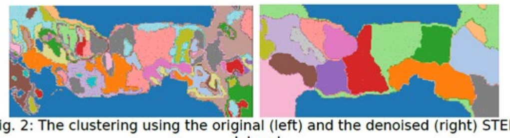

Fig. 2: The clustering using the original (left) and the denoised (right) STEM dataset

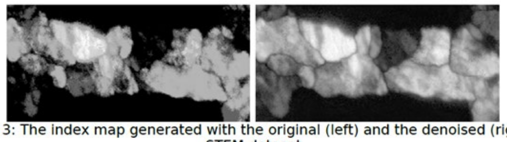

Fig. 3: The index map generated with the original (left) and the denoised (right) STEM dataset

Keywords:

4D-STEM, Denoising, Machine Learning

Reference:

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