Deep Learning-Driven Approach for Crystal Selection in Serial Electron Diffraction

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The determination of matter's properties heavily relies on understanding its structure, which plays a crucial role in various scientific domains. X-ray crystallography has conventionally been the primary technique for examining atomic arrangements, however, challenges in obtaining suitable crystals have led to the emergence of alternative methods. Electron diffraction (ED) has shown promise as a technique capable of probing atomic arrangements in small crystals, making it particularly suited for nanomaterials, thin films, and disordered materials.

One major challenge in single-crystal techniques is the sensitivity of the sample to the electron beam, which limits the acquisition of complete information. Serial crystallography offers a solution to this problem by collecting diffraction patterns from randomly oriented crystals in a large ensemble on the grid. This approach allows for the use of higher beam energy for each crystal, resulting in a higher signal-to-noise ratio compared to traditional methods.

Serial electron diffraction (SerialED), introduced by Smeets et al. in 2018 [2], involves mapping a sample consisting of nanocrystals using wide-field TEM mode. To achieve data completeness for structural studies, hundreds to thousands of diffraction patterns are collected during a SerialED experiment. Therefore, an efficient automatic data collection pipeline is essential.

Currently, threshold methods are used to automatically find crystals [2,3]. While these algorithms are unbiased, the contrast of the lacey carbon grid can affect the results. The lacey carbon film's special configuration is characterized by an array of randomly distributed holes. This type of carbon film is the most widely used in material science. To address this issue, we propose a novel approach using neural network-assisted algorithms. However, due to the diverse shapes of crystals in material science, training a generalized model would require a vast amount of data from different samples.

Our solution involves training a model to identify the carbon film on each image, allowing us to remove it and facilitate accurate crystal detection using thresholding. This approach makes SerialED more user-friendly and time-efficient, enabling researchers to analyze crystal structures of sensitive materials and perform phase analysis. To train the machine learning algorithm, a large dataset of crystal images obtained from real experiments will be utilized. This dataset will include images taken by different people, introducing variability in imaging conditions, perspectives, and styles. Incorporating images captured by multiple individuals will enhance the algorithm's ability to generalize and adapt to different experimental setups, making it more robust and effective in real-world scenarios.

In summary, the utilization of machine learning to automate crystal detection and selection in serial electron diffraction offers several advantages, including reduced electron dose to the sample, quick and accurate data processing, and high-throughput screening of crystals. This advancement has the potential to accelerate the discovery of new materials and enhance our understanding of their properties.


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