# Exploring Techniques for Diffraction Ring Detection in Molecular Research

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## Background

A substantial amount of visual data is created while conducting single-molecule experiments, and there is a notable gap in algorithms specifically designed for analysing visual data from magnetic tweezers experiments. Existing algorithms, when available, often have significant limitations such as not being able to track a moving bead accurately. Moreover, they **require expensive, specialised equipment purchases, which limits accessibility.**

## Experiment Data

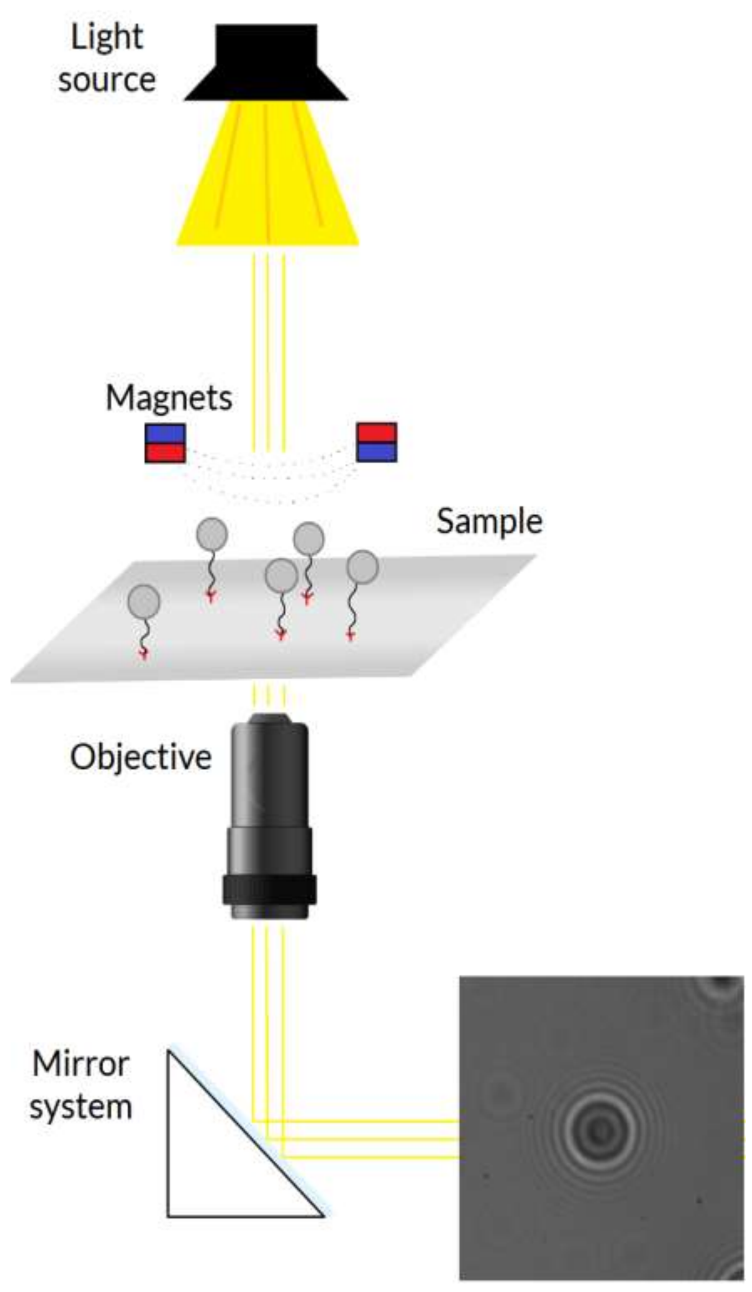


Fig. 1. Experiment data acquisition.

The figure (Fig.1.) presents a schematic of the experimental setup for a magnetic tweezers experiment. The sample is observed using microscopy. A light source is positioned above the sample, while an objective lens is located below it. The sample is placed within a flow cell - a small channel between two microscopic glass slides - filled with a buffer solution that meets the experimental conditions. The light signal passing through the sample and the optical objective is directed to a camera via a system of mirrors.

## Workflow

To reduce noise and artifacts, we applied a series of image transformations, starting with a Fourier transform to shift the image into the frequency domain, followed by a bandpass filter to remove irrelevant low and high frequencies. The inverse Fourier transform was then applied to return the image to the spatial domain. Intensity profile peak detection was used to locate diffraction rings, while frame interpolation ensured consistency across frames. Finally, movement-dependent smoothing was employed to reduce residual noise and fluctuations, thereby improving the accuracy of the diffraction ring tracking.

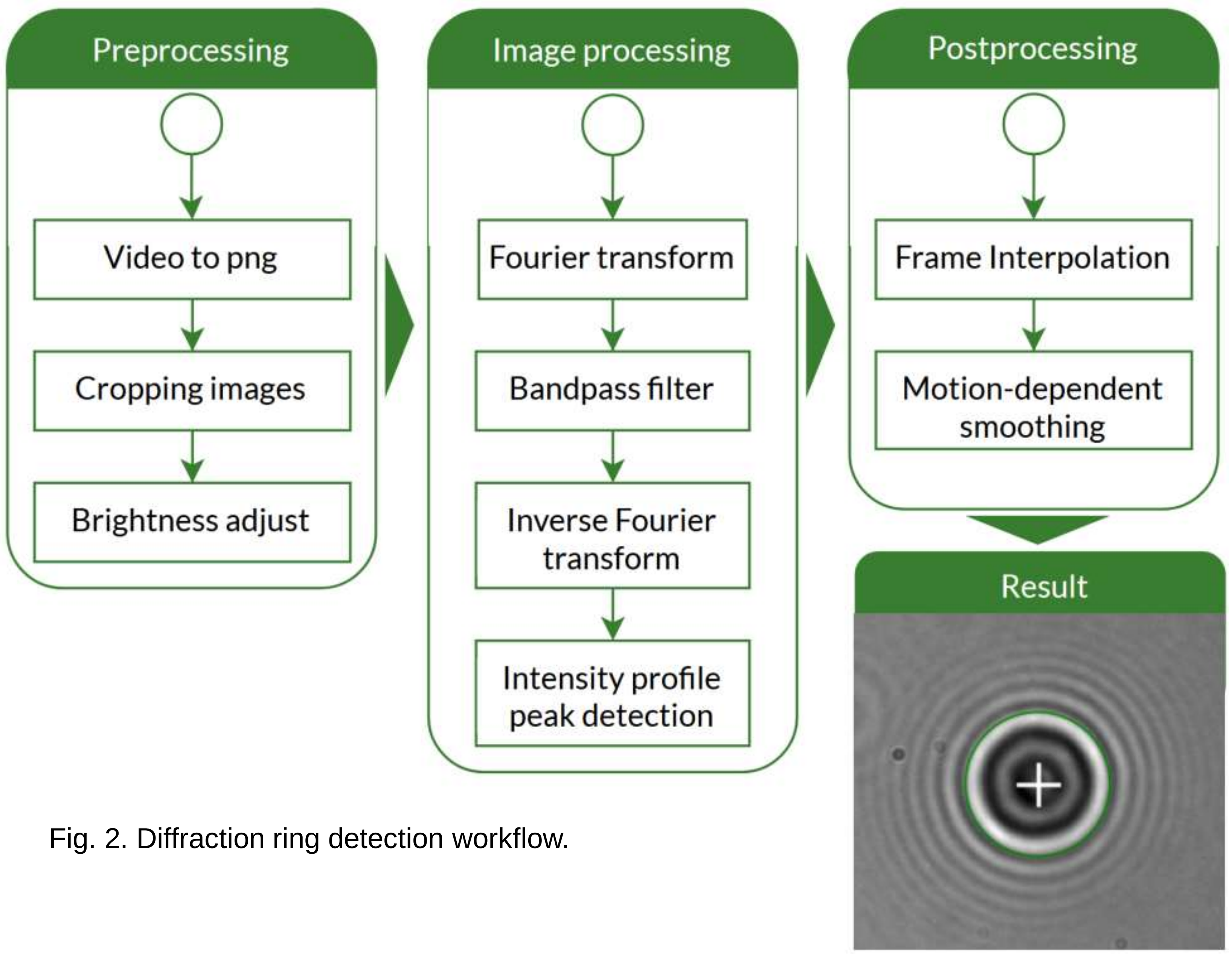


Fig. 2. Diffraction ring detection workflow.

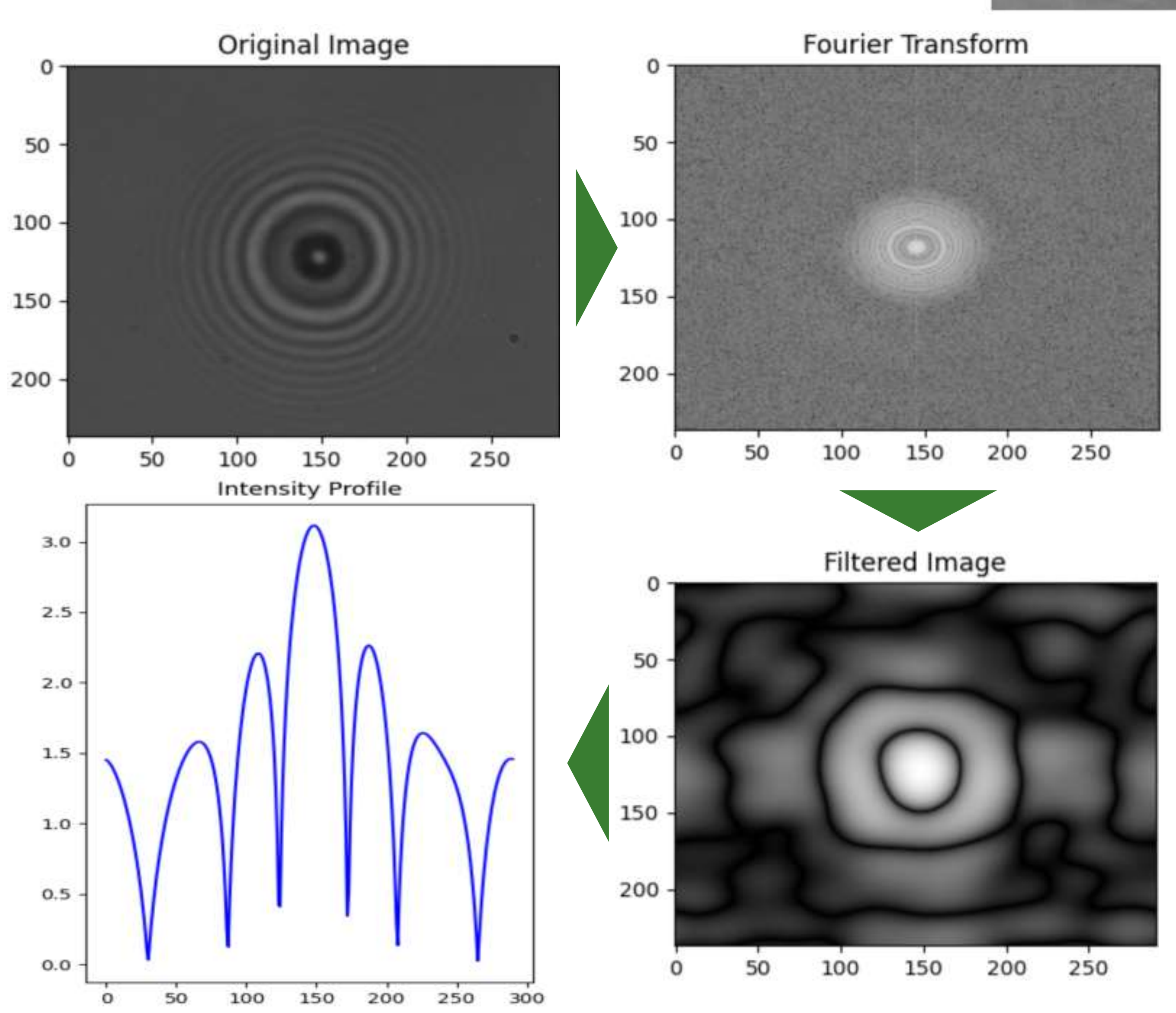


Fig. 3. Visual representation of the image processing steps taken.

## Results

Across 10 validation videos, each consisting of 50 frames, our algorithm successfully identified difraction rings in 233 frames, achieving an overall **accuracy of 46.6%.** Additionally, 9.2% of the frames demonstrated near-correct identification and tracking, highlighting the algorithm's potential, while the incorrect detection rate of 44.2% suggests areas for further improvement.

However, it has **yet to achieve the level of precision** exhibited by other existing algorithms designed for this specific area of study (Fig. 5.), deviating by fractions of a micrometer.

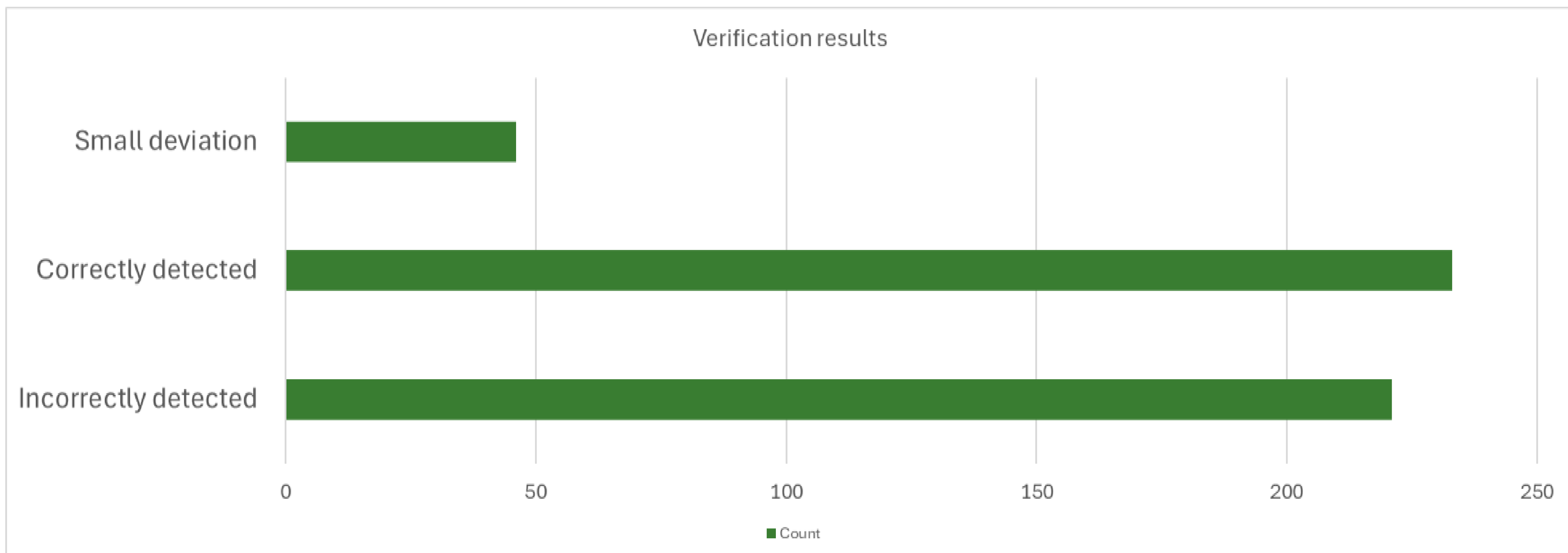


Fig. 4. Validation results of our test data.

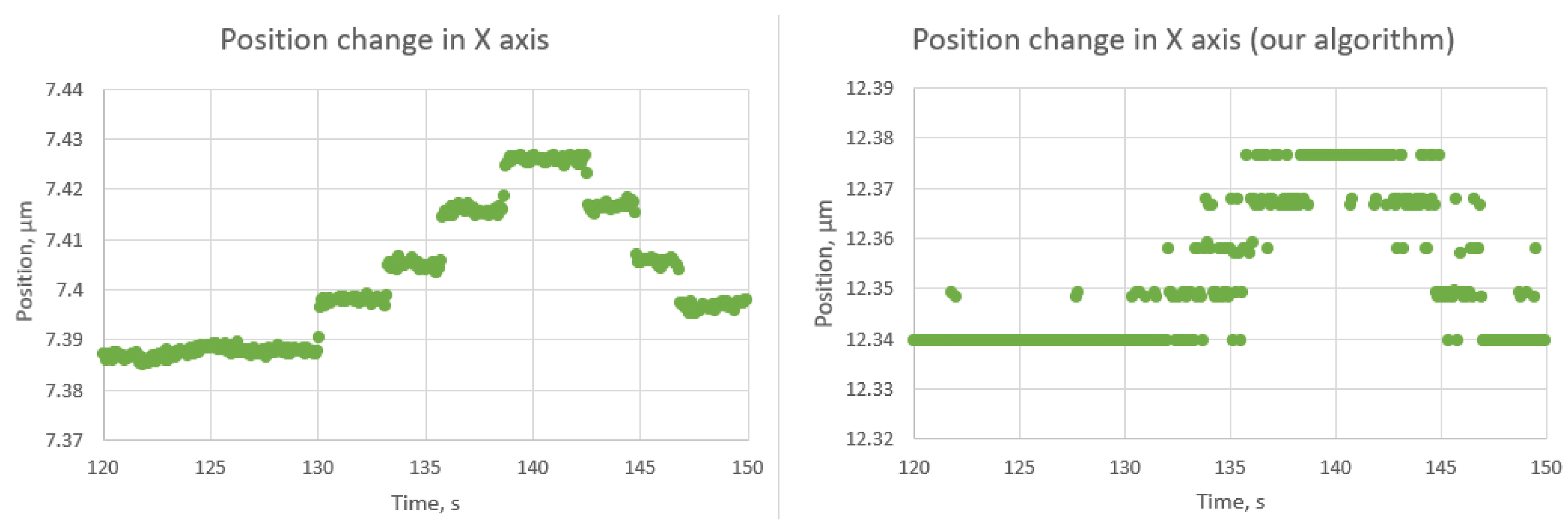


Fig. 5. Comparison with an existing algorithm (left) (developed by Ralf Seidel).

## Future Work

To improve the diffraction ring detection algorithm's performance and expand its capabilities, we propose the following avenues for future work:

- We aim to incorporate a larger and more diverse set of validation data, including videos with varied noise levels, to better assess the algorithm's robustness.
- Future testing will involve experimenting with different parameters, such as various filter sizes, to optimize diffraction ring detection in different experimental scenarios.
- By training autoencoders for feature extraction, we hope to enhance the precision of diffraction ring detection and reduce the rate of incorrect identification.

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