Automated Identification of Unit Cell Defects in Porous MOFs and Zeolites

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Introduction

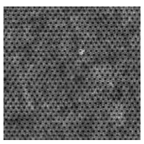
- MOFs and Zeolites are porous crystalline materials used in catalysis, gas storage and separation.
- Their properties are strongly influence by unit cell integrity and presence of defects.
- Traditional manual analysis of TEM images are time consuming, subjective and requires expert interpretation.
- Deep learning model (e.g., CNNs) face limitation, struggles with structurally similar framework and require large labeled datasets.

Objectives

- Develop an automated pipeline to identify and classify unit cell defects in MOFs and zeolites using TEM images.
- Overcome challenges of traditional machine learning by avoiding the need for labeled data, focusing on unsupervised learning.
- Enable detection of known structures (e.g., MFI, MEL) and possibly novel defect structure.

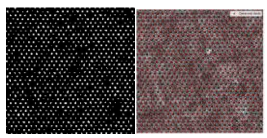
Methodology

1. Load Image



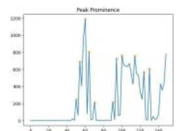
- Import Greyscale

2. Voids Detection



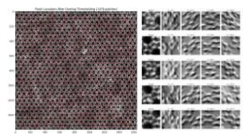
- Thresholding & Masking

3. Compute Radial Distance Frequency (RDF)



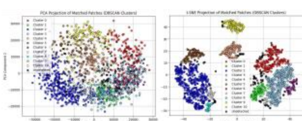
- Patch Size = Peak
- Unit Cell = Peak / 2

4. Patch Extraction & Gabor Filter Feature Extraction



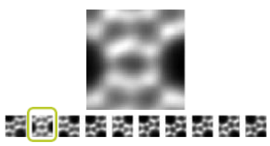
- Extract at (0°, 60°, 120°, 180°, 240°, 300°)
- 4 Gabor Filter (0°, 45°, 90°, 135°)

5. PCA Projection & t-SNE with DBSCAN Clustering



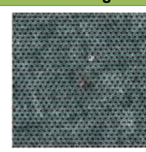
- 97% Variance Retained

6. Compute Averaged Cluster & Select Best Patch



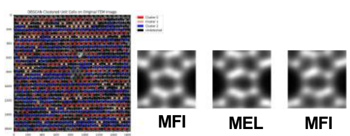
- Select Clearest Structure

7. Re-run with Template Matching



- Cross-Correlation Matching

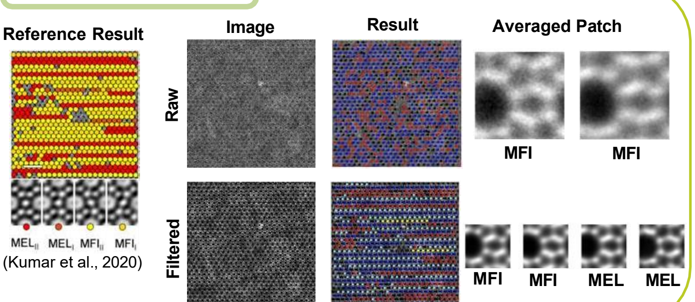
8. Result Overlay on Original TEM image



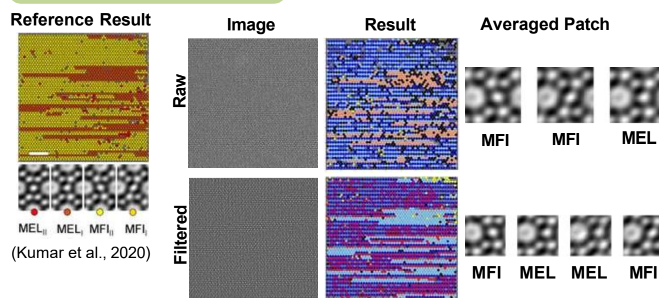
- Color Coded on TEM Image

Results and Discussion

Dark Field TEM



Bright Field TEM



Raw Images:

- Raw Images shows high noise levels and uneven contrast reduced clustering accuracy.
- Fewer voids detected, leading to larger patch size and inaccurate representation of unit cell.
- Structural details were less distinct, leading to potential misclassification.

Filtered Images:

- Improved void detection due to enhanced contrast and uniform background.
- More distinct RDF peak, resulting in more accurate patch size estimation.
- Tighter, separable group t-SNE clustering.
- Clearer averaged unit cell for both MFI and MEL.
- Improved detection with fewer undetected (black spots) cluster.

Conclusion

- Preprocessing and filtering play a critical role in improving the downstream analysis.
- Improvement in signal-to-noise ratio allows for more reliable unsupervised clustering and defect detection.
- The comparison between raw and filtered images demonstrated the method's robustness across different imaging mode and image qualities.

References

1. Kumar, P., Kim, D. W., Rangnekar, N., Xu, H., Fetisov, E. O., Ghosh, S., Zhang, H., Xiao, Q., Shete, M., Siepmann, J. I., Dumitrica, T., McCool, B., Tsapatsis, M., & Mkhoyan, K. A. (2020). One-dimensional intergrowths in two-dimensional zeolite nanosheets and their effect on ultra-selective transport. *Nature Materials*, *19*(4), 443–449. https://doi.org/10.1038/s41563-019-0581-3