Symmetry-Aware Deep Learning for Generalizable STEM Phase Classification

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1. Introduction

Accurate and rapid identification of structural phases from atomically resolved scanning transmission electron microscopy (STEM) images is essential for understanding structure-property relationships in materials science. While deep learning models have shown promise for classifying and segmenting material phases[1], they often fail to generalize beyond their training distribution—networks trained on one material frequently underperform when applied to novel structures, limiting their utility in materials discovery.

This limitation stems from the extraordinary diversity of crystal structures. Materials span hundreds of space groups with distinct symmetries[2], and real samples exhibit defects, grain boundaries, and compositional variations. Such structural complexity makes it impractical to curate training datasets that adequately represent all possible atomic configurations. Compounding this challenge, no large-scale foundation dataset exists for STEM-based phase identification—unlike ImageNet for natural images, there is no equivalent repository of labeled atomic-resolution micrographs spanning diverse material systems. As a result, models trained on limited data from specific materials cannot reliably recognize phases with unfamiliar symmetries, lattice parameters, or atomic arrangements. This out-of-distribution problem fundamentally restricts the deployment of current deep learning approaches for automated, high-throughput phase screening in exploratory materials research.

In this work, we address this generalization challenge by incorporating local symmetry information as material-agnostic features for phase identification.

2. Symmetry maps as additional features

Symmetry is an intrinsic property of crystal structures, independent of chemical composition or lattice parameters. Leveraging this universality, we use Zernike polynomials to compute rotational and reflectional symmetry maps directly from STEM images [3]. These maps encode local symmetry information as additional input channels alongside raw pixel intensities, providing the model with physics-informed features that generalize across chemically distinct systems. Figure 1 displays a representative STEM image of $MoSe_2$ alongside its corresponding symmetry maps that quantify the degree of local rotational and mirror symmetry at each pixel. By explicitly encoding symmetry, we reduce the effective complexity of the input space, allowing the model to recognize shared structural motifs across chemically diverse materials.

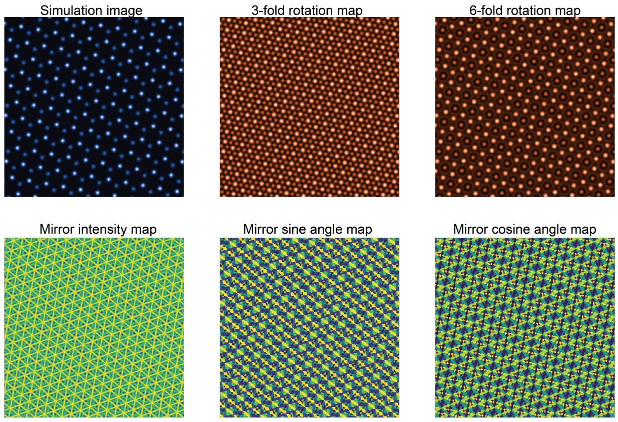

Fig. 1: An atomic resolution STEM image of $MoSe_2$ and corresponding symmetry maps. The first row shows simulation image (in blue) and rotational symmetry maps (in orange): a 3-fold map (middle) and a 6-fold map (right). The second row presents reflectional symmetry maps: a reflectional intensity map (left), followed by sine and cosine maps representing mirror orientations.

3. Symmetry-aware framework

We demonstrate the effectiveness of incorporating symmetry channels by training multiple classifiers on simulated plane group images. Without symmetry information, classifiers achieve only 45.3% accuracy on unseen structures. In contrast, classifiers trained with symmetry information achieve 96% accuracy, representing a more than 2-fold improvement in cross-material generalization. Figure 2 illustrates the framework for this workflow.

Our results show that integrating symmetry context enables a single model to generalize across diverse materials, overcoming the out-of-distribution challenges that limit conventional deep neural networks. This work advances deep learning for microscopy by shifting from task-specific models toward a unified framework for structural and defect classification across varied material systems—a critical step toward foundation models for atomic-resolution microscopy.

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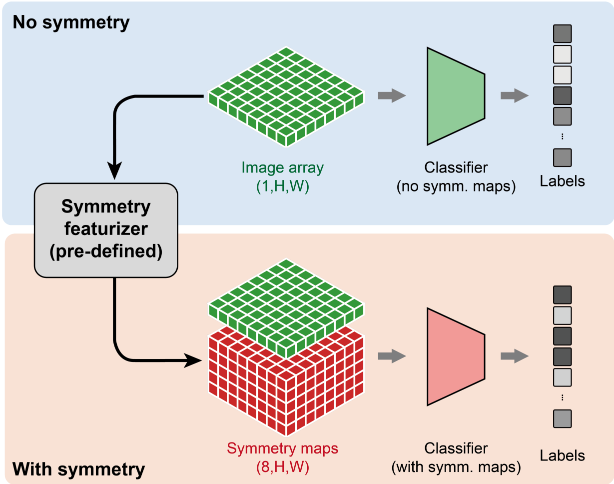

Fig. 2: Framework for training a generalized phase-classification model using atomic images and symmetry maps. The process compares two approaches. The upper path (blue) classifies structural phases using atomic-resolution images alone. The lower path (orange) enhances classification by integrating both atomic images and their corresponding symmetry maps, which significantly improve model's ability to generalize across materials.

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