Understanding Experimental Images by Identifying Symmetries with Deep Learning

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1. Wallpaper Group Symmetry Datasets

- Three distinct datasets: **ImageNet Symmetry dataset,[1] Atom Symmetry dataset, Noise Symmetry dataset.**
- Construct primitive unit cell to translation unit cell in shapes: **square, rectangle, rhombic shape, oblique shape,** and **hexagon.**
- Area size of the translation unit cell unit cell is randomly distributed within a defined range.
- Image construction steps: symmetry operation such as **rotation, mirroring,** and **glide** on primitive unit cell, then translated and padded to attain a predetermined image size to ensure uniformity.
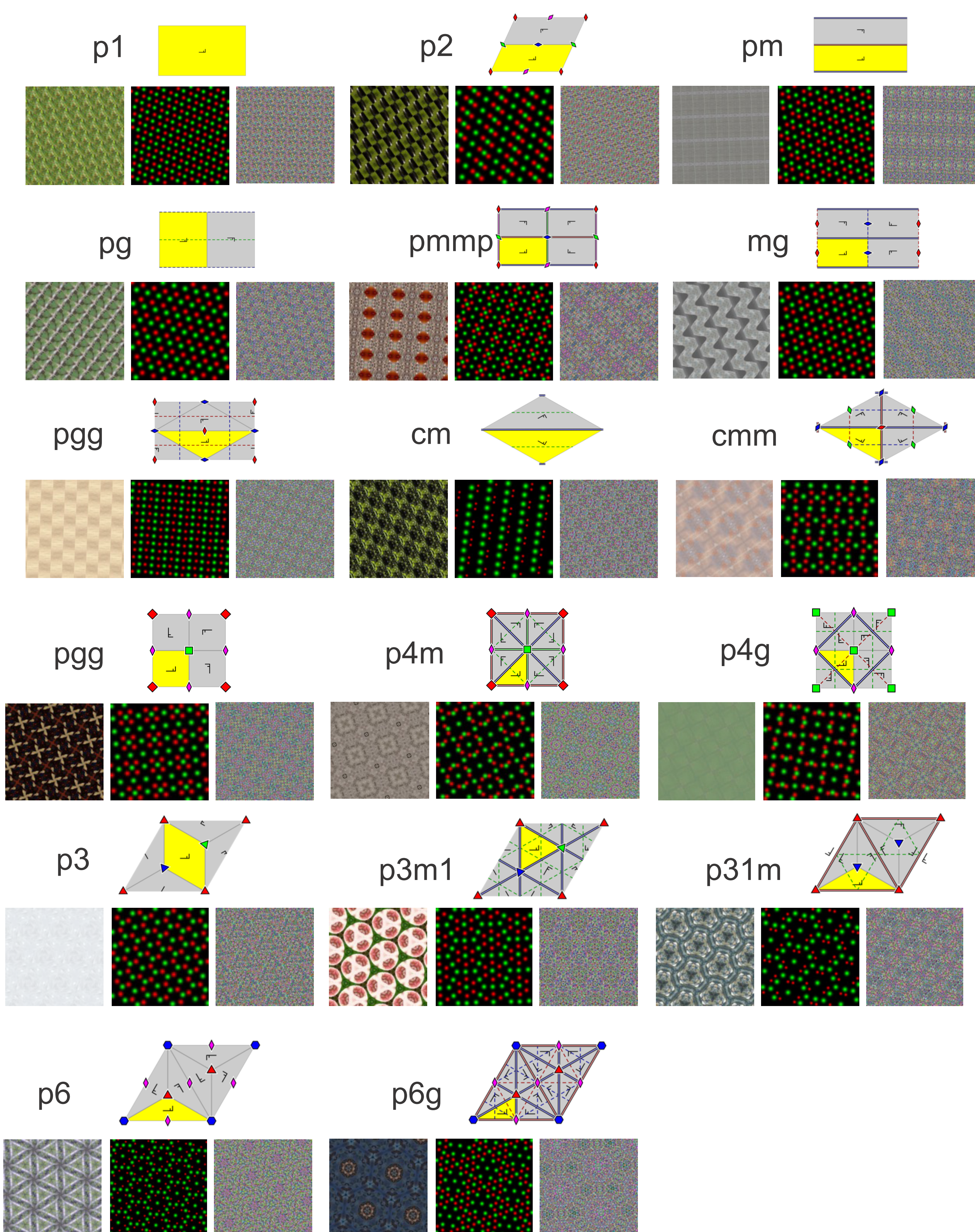

2. Benchmark Results

Model	Accuracy			Loss		
	Train	Valid	Test	Train	Valid	Test
ResNet50 [2]	99.96%	99.91%	54.33%	0.0011	0.0037	6.188
DenseNet161 [3]	99.94%	99.93%	58.69%	0.0012	0.0042	5.856
FPN_ResNet50 [4]	99.94%	99.91%	52.59%	0.0017	0.0031	4.312
XCiT [5]	99.96%	99.90%	45.00%	0.0010	0.0061	10.116

Confusion Matrix of Atom Symmetry Dataset (Testing Set)
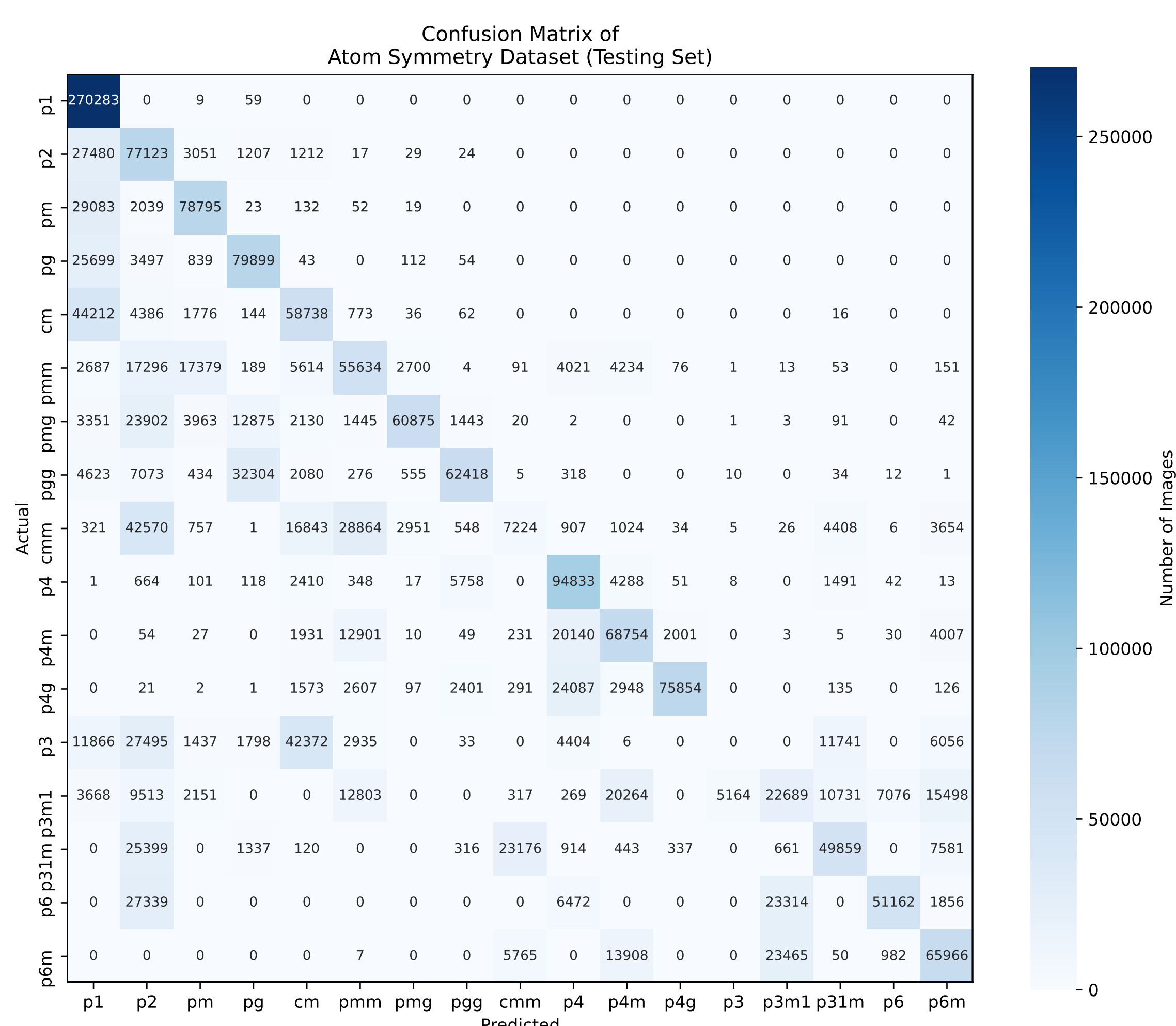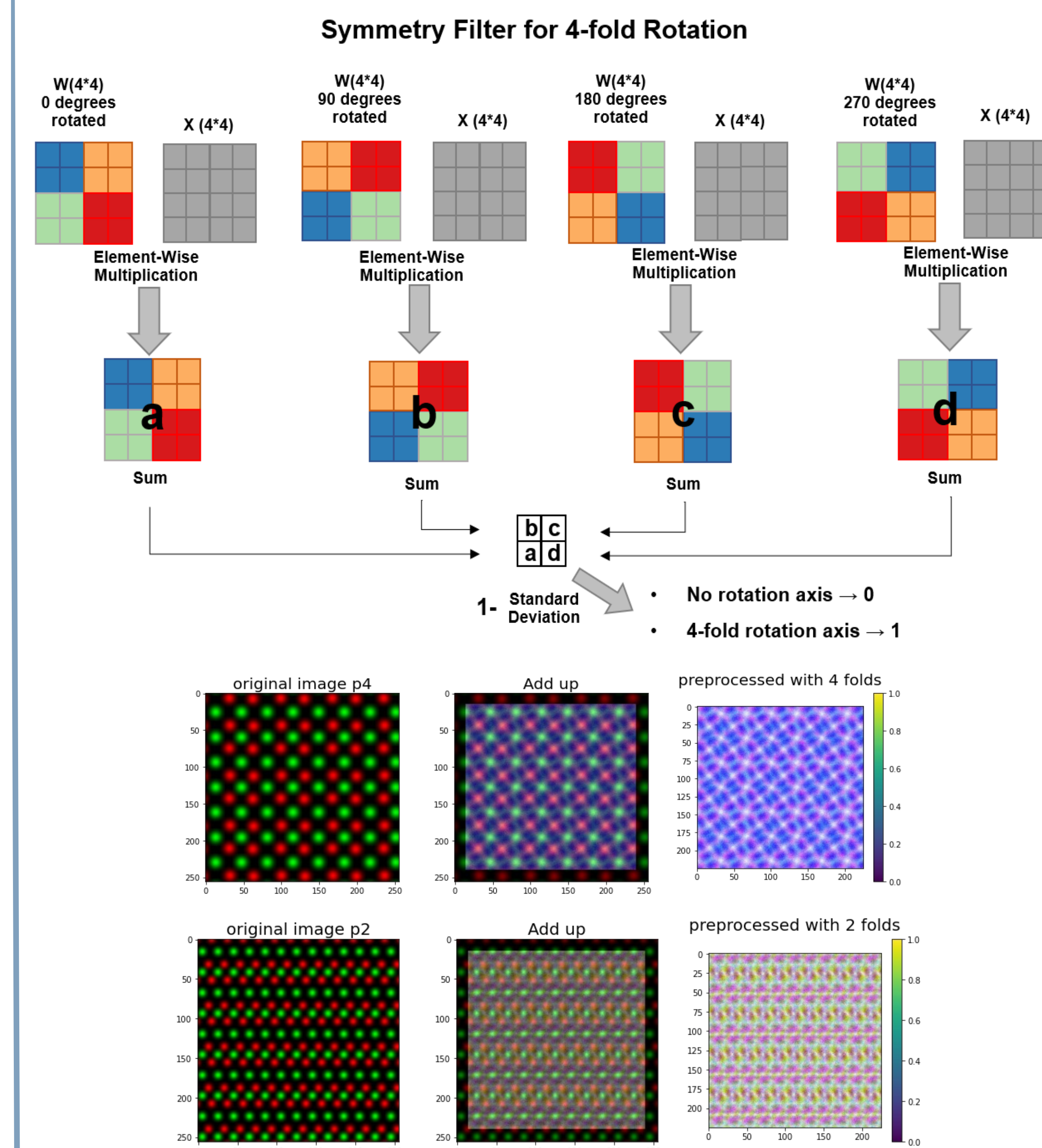
3. Design of Training Workflow

Hierarchy structure of wallpaper group symmetries:
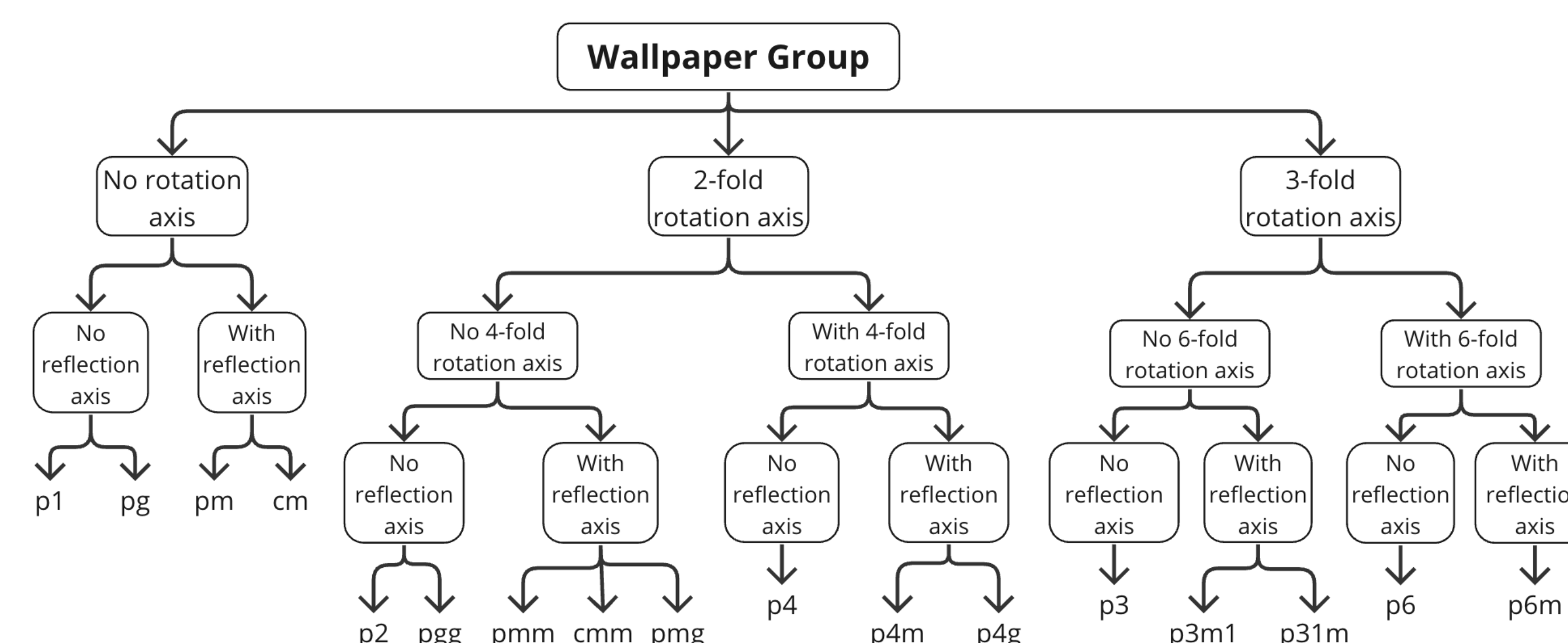
Classification for level 1 of hierarchy dataset - classification:
No rotation axis, 2-fold rotation axis, 3-fold rotation axis

Training accuracy: 99.98%; validation accuracy: 96.18%; cross-validation accuracy: 48.7%.

4. Data Preprocessing with Equivariance

Symmetry Filter for 4-fold Rotation

- No rotation axis → 0
- 4-fold rotation axis → 1

5. Future Work

1. Implement customized symmetry filter in deep learning model to identify symmetry in a effecgive and robust way.
2. Design training workflow to better guide model to identify symmetry in hierarchy manner.
3. Explore possible solution for symmetry idensification by enable equivariance in convolutional layers based on recent studies.[6-9]

Dataset:
Due to the size limit, a subset of dataset is available at **Zenodo - *DOI: 10.5281/zenodo.7384734.*** Full dataset (10 million) is available upon request.

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