# Symmetry quantification and segmentation in STEM imaging through Zernike moments

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## Background: Symmetry Quantification in STEM

We present a method using Zernike moments[1] for quantifying rotational and reflectional symmetries in scanning transmission electron microscopy (STEM) images[2], aimed at enhancing atomic-scale structural analysis. This technique is resilient to common imaging noise, making it suitable for low-dose imaging and identifying quantum defects. We demonstrate its utility in unsupervised segmentation of polytypes in twisted bilayer $TaS_2$, enabling precise differentiation of structural phases and monitoring transitions induced by electron beam effects.

**Challenges**:

**Noise Resilience:** Ensuring effectiveness against diverse imaging noise, particularly in low-dose conditions.
**Scalability:** Adapting the method for large datasets or complex structures while maintaining efficiency.

**Contributions**:

**Symmetry Quantification:** Novel method for quantifying symmetries in STEM images, improving structural analysis.
**Segmentation Accuracy:** Accurate segmentation of polytypes in twisted bilayer $TaS_2$, offering insights into structural phases and their transitions.

## Representation of patches as Zernike moments

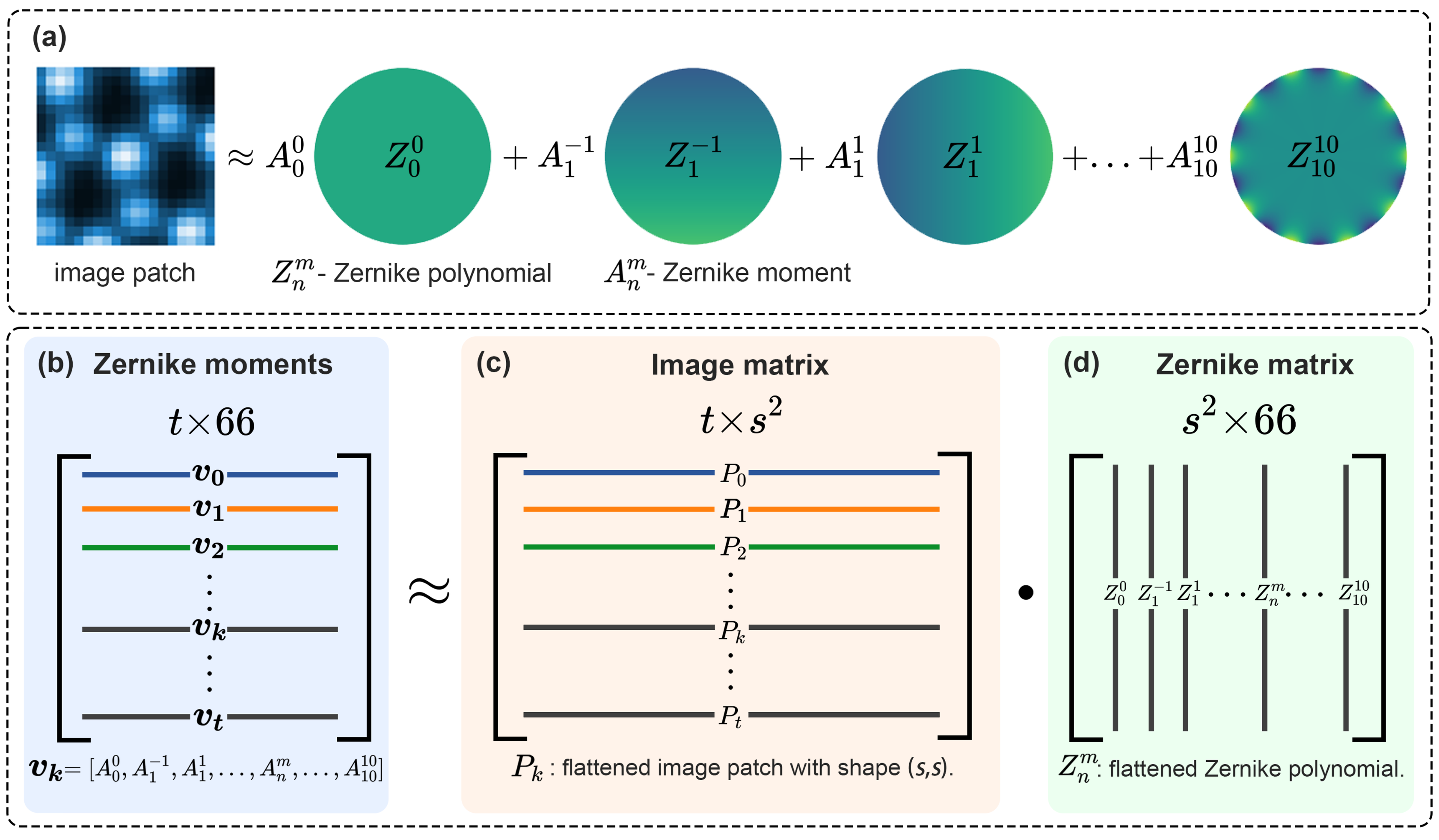


Figure 1. Representation of image patches as Zernike moments. (a) depicts the approximation of an image patch (left) as a linear combination of Zernike polynomials $Z_n^m$ with coefficient $A_n^m$, which is called Zernike moment. Zernike moments can be calculated via dot product, as shown from (b) to (d).

## *N*-fold rotational symmetry score, $S_N$

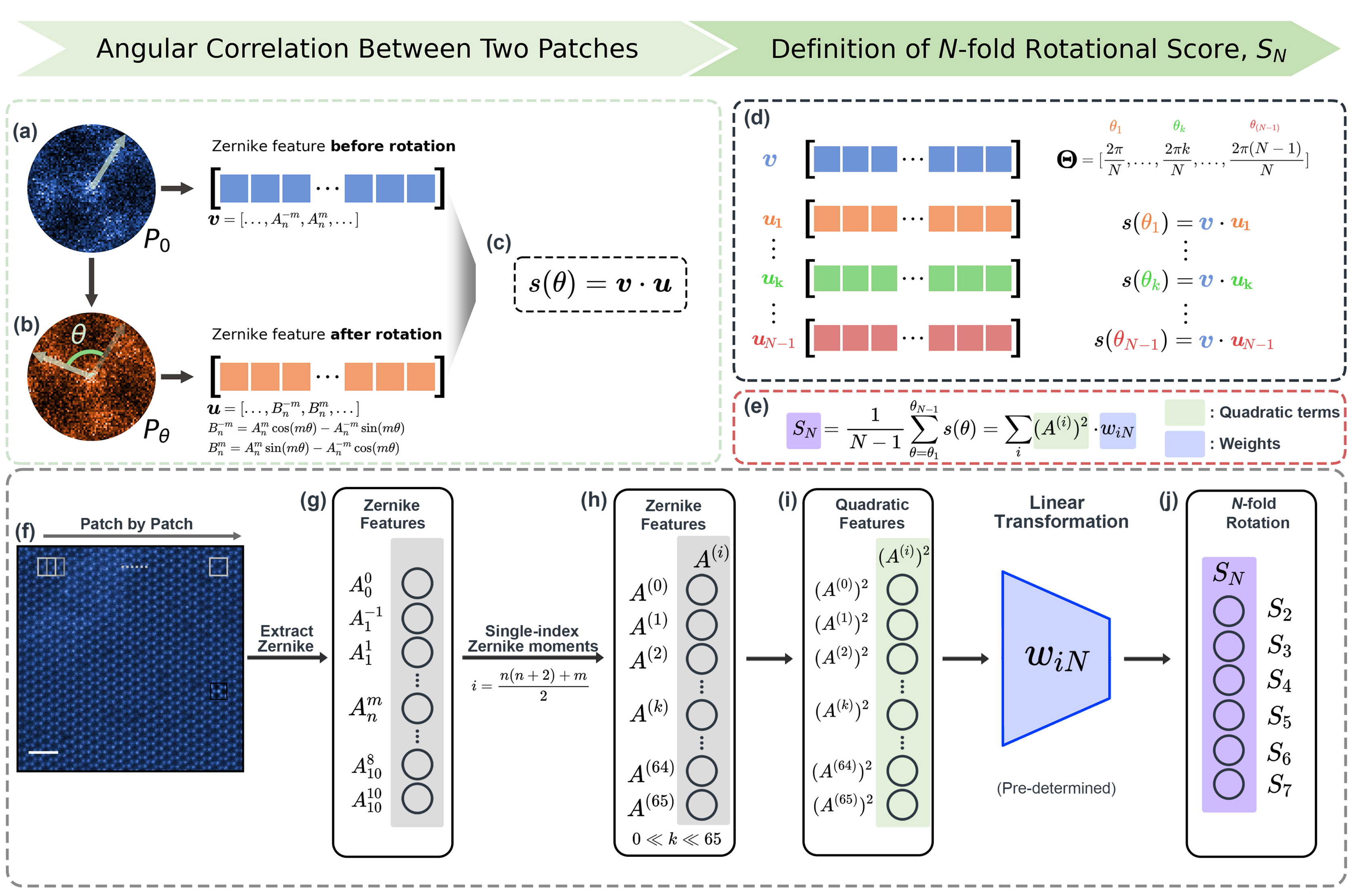


Figure 2. Illustration of *N*-fold rotational symmetry score $S_N$. (a) Original HAADF-STEM image patch ($P_0$) and its Zernike feature vector $\boldsymbol{v}$. (b) Rotated patch ($P_\theta$) and corresponding Zernike vector $\boldsymbol{u}$. (c) Similarity score $s(\theta)$ from dot product of $\boldsymbol{v}$ and $\boldsymbol{u}$. (d) Series of similarity scores for discrete rotation angles $\boldsymbol{\Theta}$. (e) Mean similarity score defines $S_N$. (f) Local patches via sliding window technique. (g) First 66 Zernike moments for each patch. (h) Conversion of Zernike moments to single index format. (i) Squaring Zernike features. (j) $S_N$ as a linear combination of quadratic terms with coefficients $w_{iN}$. (Scale bar: 1 nm)

## Reflectional symmetry score, $S_R$

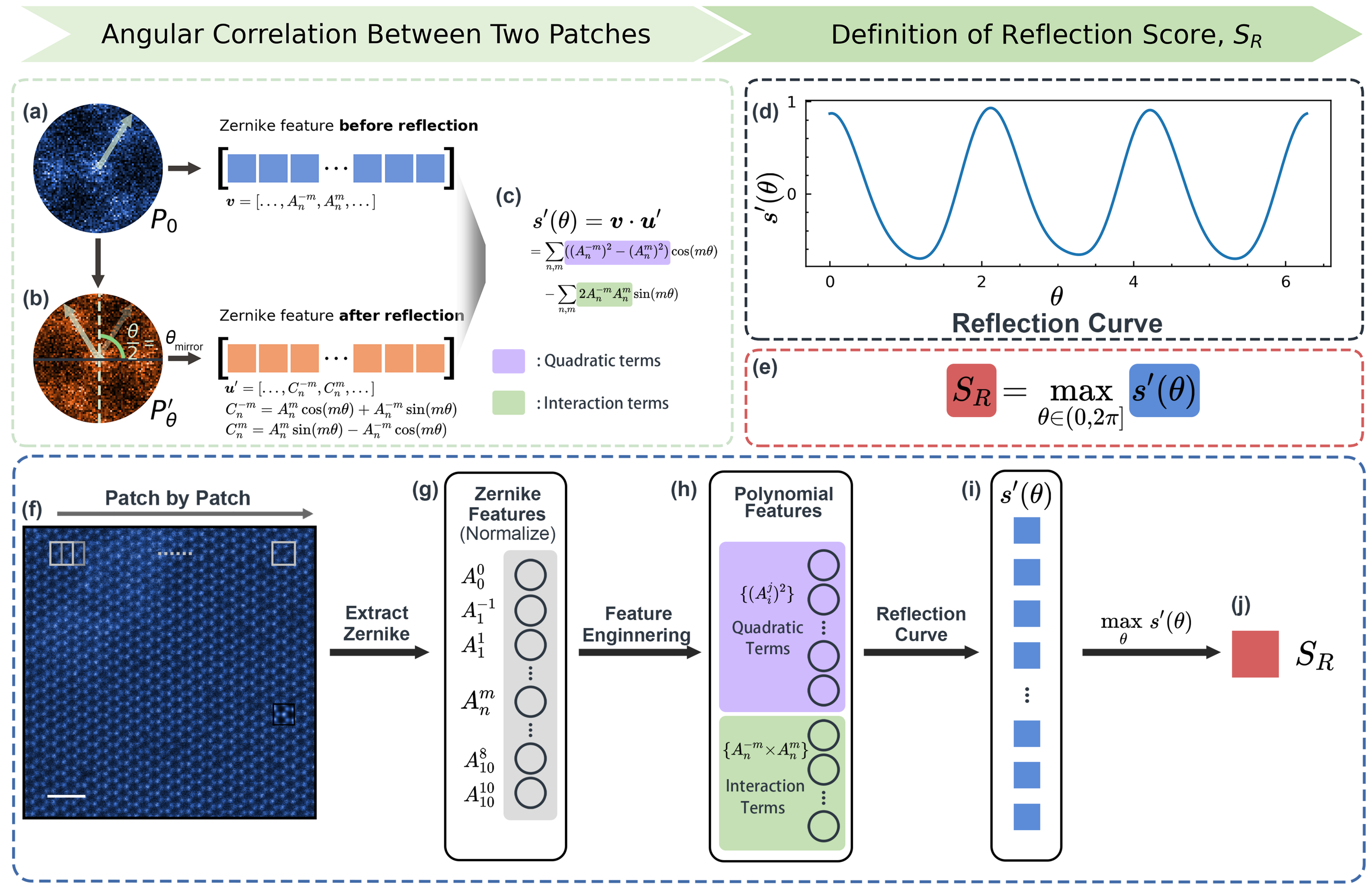


Figure 3. Illustration of reflectional symmetry score $S_R$. (a) Original HAADF-STEM image patch ($P_0$) and its Zernike feature vector $\boldsymbol{v}$. (b) Reflected patch ($P'_\theta$) and its Zernike vector $\boldsymbol{u}'$. (c) Similarity score $s'(\theta)$ from dot product of $\boldsymbol{v}$ and $\boldsymbol{u}'$. (d) Reflectional curve $s'(\theta)$ for continuous angles $\theta$. (e) Reflectional score $S_R$ is the maximum value of $s'(\theta)$. (f) Local patches via sliding window technique. (g) First 66 Zernike moments for each patch. (h) Calculation of the reflectional curve $s'(\theta)$. (i) Visualization of reflection curve. (j) Maximum of $s'(\theta)$ defines $S_R$. (Scale bar: 1 nm)

## Rotational and reflectional symmetry maps

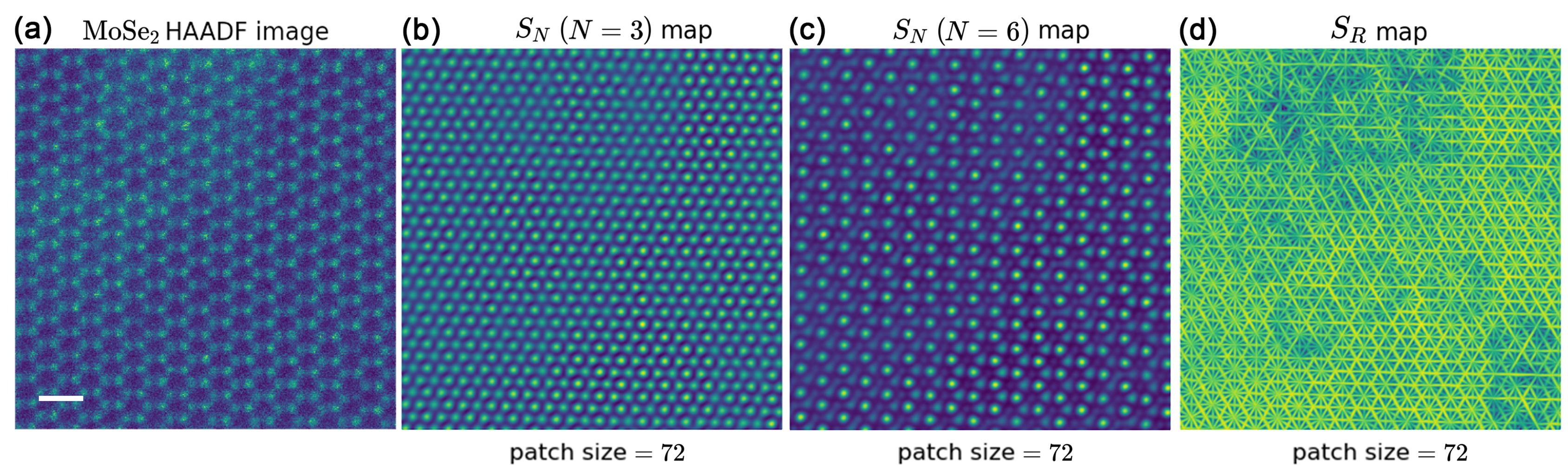


Figure 4. Rotational and reflectional symmetry maps of an experimental monolayer $MoSe_2$ HAADF image. (a) depicts the experimental HAADF-STEM image of a monolayer $MoSe_2$ with defects and contamination (upper left). (b)–(d) 3-fold, 6-fold, and reflectional symmetry maps calculated from the experimental image in panel a. (scale bar: 0.5 nm)

## Segmentation in twisted bilayer $TaS_2$

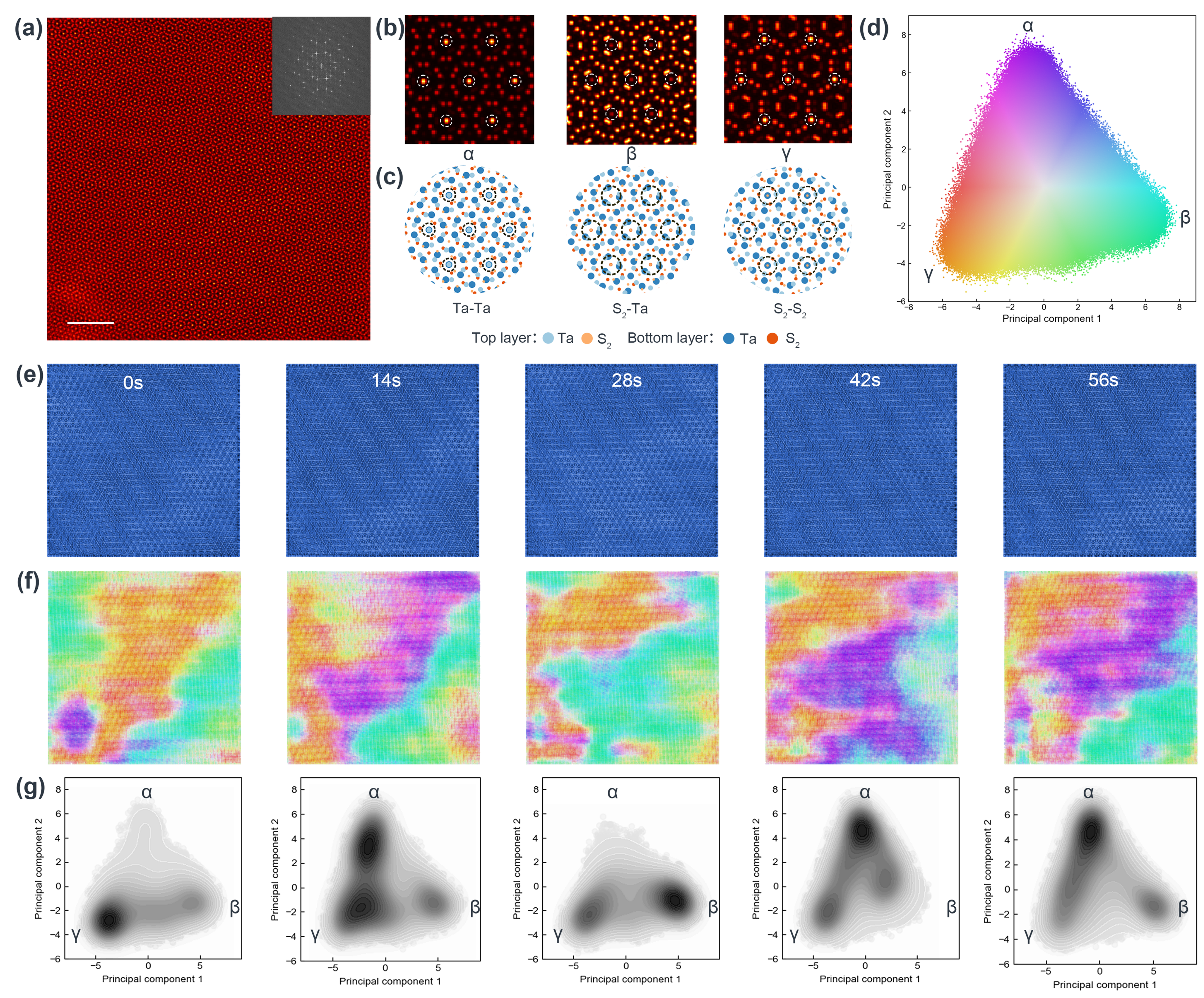


Figure 5. Reflectional symmetry maps delineate phases in twisted bilayer $TaS_2$. (a) Experimental HAADF-STEM image and FFT (power spectrum) of twisted bilayer $TaS_2$. (b) Multislice simulation images of $\alpha$-, $\beta$-, and $\gamma$-$TaS_2$ stacking phases. (c) Atomic structures of phases from panel b. (d) 2D PCA layout of local FFT patterns from reflectional symmetry maps in panel e. (e) Reflectional symmetry map of HAADF-STEM images across time series. (f) Phase segmentation based on reflectional symmetry maps in panel e. (g) Density plots of phases in 2D PCA space, with the same principal components as in panel d. (Scale bar: 4 nm)

## References

[1] Dan, J. et al., **Science Advances 8** (2022), doi:10.1126/sciadv.abk1005
[2] Dan, J. et al., **Chinese Physics B** (**2024**), doi:10.1088/1674-1056/ad51f4
[3] GitHub repository – motif-learn: https://github.com/jiadongdan/motif-learn

motif-learn