Poster

Detecting and Correcting Systematic STM Imaging Errors: Plane Symmetry of Graphite Calibration Samples

T. Bortel[1], A. P. Baddorf[2], R. K. Vasudevan[2], P. Moeck[1*]
[1] *Nano-Crystallography Group, Department of Physics, Portland State University, Portland/OR, USA*
[2] *Center for Nanophase Materials Sciences,‡ Oak Ridge National Laboratory, Oak Ridge/TN, USA*
* *pmoeck@pdx.edu*

When capturing atomic resolution imagery, such as that taken via scanning tunnelling microscopy (STM), systematic errors are not unusual. For example, a sample and probing tip are moved relative to each other in STM by piezoelectric actuators. These actuators often have the shape of a tube and allow for both sample movements up to hundreds of nanometers while selecting scanning areas and scanning at high precision. This necessitates relatively large bending of the tube to scan peripheral sample areas, resulting in non-linear piezoelectric responses and sample drift. The scanned area of the sample may then have the shape of a “skewed parallelogram”, whereas a square or rectangular image area is displayed to the operator. The resulting systematic errors can be detected by means of the quantification of symmetry breakings in such images from crystalline calibration samples such as highly-ordered pyrolytic graphite (HOPG), see Fig. 1a. As the calibration process can be complex, many publications forgo correcting for plane symmetry breakings, possibly leading to some “untenable conclusions” about the sample [1] being drawn from compromised image data.

Novel techniques have recently emerged for measuring and categorizing two-dimensional (2D) symmetries in noisy digital crystal images with atomic (or molecular) resolution [2, 3]. The methods in question do not rely on a particular imaging technique and are thus agnostic to the particulars of any given microscope or imaging technique. The results of the methods are classifications into Bravais lattice types, projected Laue classes, plane symmetry groups, and the associated site symmetries. Because the methods rely on geometric Akaike Information Criteria [4] instead of subjective/arbitrary thresholds, the resultant classifications are an *objective* description of the symmetry that has been transferred from an ideal crystalline sample through the microscope to its real digital image.

We present a methodology for detecting and correcting these sorts of errors based on ideas of Henriksen and Stipp [1] and our own methods for classifications into plane symmetry groups. First, symmetries are detected and objectively classified from the complex translation-periodic Fourier coefficients of the original image [2, 3]. The $J_{x...}$ values in Fig. 1 are squared residuals for minimal supergroups and maximal subgroups (of plane symmetry groups) respectively. Their ratios identify the group that is maximally supported by the experimental data. Afterwards, calculations are performed in Fourier space to determine the correct linear transformation to be applied to the original image in direct space. Once the correction has been applied, the objective plane symmetry group classification confirms that the symmetry of the STM image, Fig. 1b is indeed that of the HOPG calibration sample. The necessary computer code to apply such corrections to digital images from hexagonal crystals will be made freely available on GitHub.

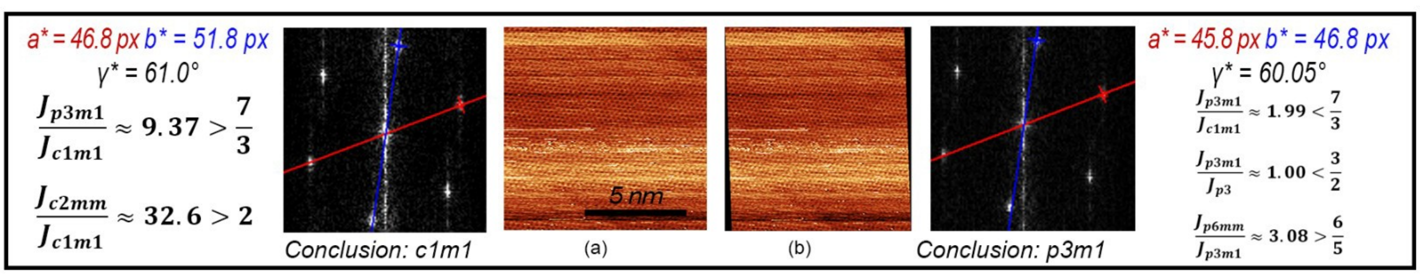

Figure 1. HOPG imaged at the "NanoTransport“ STM [5] of the Oak Ridge National Laboratory by the authors in 2022 before (**a-** left-center) and after (**b**-right-center) applying the derived affine distortion in direct space that counteracts the imaging-induced distortions in the original image. Further to the flanks of the figure are the discrete Fourier transforms of the respective images and measurements taken from those transforms. Note that the determined plane symmetry group of the images changes from *c1m1* to *p3m1* as result of the direct space transformation. (The reciprocal lattice vector magnitudes are in units of pixels in Fourier space.)

[1] K. Henriksen and S. L. S. Stipp. (2002) *American Mineralogist* **87**, 5.
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[5] https://www.ornl.gov/content/nanotransport-system.

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