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Advances in Crystallographic Image Processing for Scanning Probe Microscopy

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Advances in Crystallographic Image Processing for Scanning Probe Microscopy

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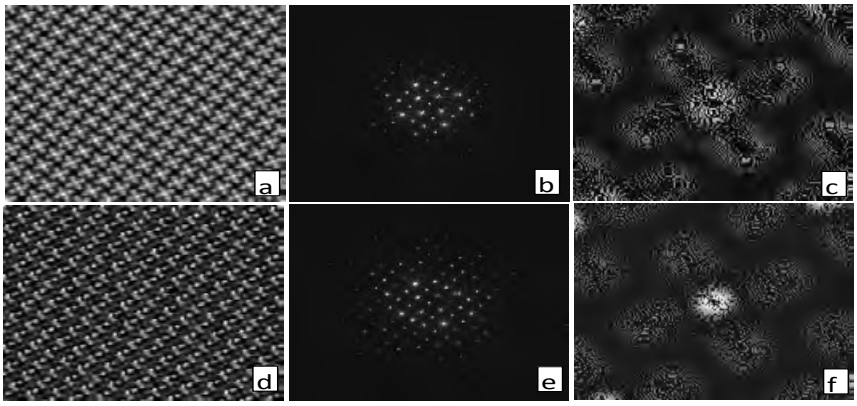
Crystallographic image processing (CIP) is well established in the electron microscopy community, where it is used for the analysis and enhancement of high-resolution transmission electron microscope images of crystals and two-dimensional (2D) arrays of membrane proteins. The technique has recently been adapted to the processing of 2D periodic images from scanning probe microscopes (SPMs) [1]. Within this context, a procedure for the unambiguous identification of the underlying Bravais lattice of an experimental or theoretical image of a 2D periodic array of objects (e.g. molecules or atoms and their respective electron density distribution functions, …) has been developed [2]. This procedure constitutes a partial solution to a longstanding but unresolved issue in CIP. The unresolved issue itself is the complete quantification of the deviations of 2D periodic images from the plane symmetry groups. A complete solution to this problem will allow for unambiguous decisions as to which plane symmetry best models experimental data when all systematic errors in the acquiring and processing of the image data have been accounted for at a level that systematic rest errors are negligible. Our 2D Bravais lattice identification procedure is independent of which type of microscope has been utilized for the recording of the images. It is based on classification procedures for non-disjoint models from the robotics community and is particularly useful for the correction of scanning tunneling microscope (STM) images that suffer from a blunt scanning probe tip artifact [2]. With the crystallographic processing of two molecular resolution STM images of periodic arrays of tetraphenoxyphthalocyanine on graphite, it is demonstrated how the classical CIP plane symmetry estimation procedures are augmented by our unambiguous translation symmetry identification method. We also apply CIP to an artificial SPM image that features a blunt scanning probe tip artifact, see the figure below.

[1] *http://www.formatex.info/microscopy4/1951-1962.pdf, http://nanocrystallography.research.pdx.edu/media/thesis14acorr.pdf, http://www.microscopy.org/MandM/2010/plachinda.pdf, http://nanocrystallography.research.pdx.edu/media/cms _page_media/6/Taylor_thesis_,*
[2] *J. C. Straton, T. T. Bilyeu, B. Moon, and P. Moeck, Cryst. Res. Technol. 2014, special issue "Advances in Structural and Chemical Imaging", edited by P. Moeck and A. Holzenburg, in press*



Removal of a blunt scanning probe tip artifact by Crystallographic Image Processing (CIP). (a) Artificial SPM image of a 2D periodic array of four-leaf clover shaped objects as a sharp (single) scanning probe tip would record it. **(b)** Fourier transform amplitude map of (a). **(c)** Approximately two unit cells of (a) in a 32 level contour plot. **(d)** Artificial SPM image of a 2D periodic array of four-leaf clover shaped objects as a blunt scanning probe tip (that consists of three mini-tips) would record it. **(e)** Fourier transform amplitude map of (d). **(f)** Approximately two unit cells ***of the CIP processed version of (d)*** in a 32 level contour plot. Note the similarity between the direct space images (c) and (f), which demonstrates the removal of the blunt tip artifact. Note also that the (reciprocal) 2D lattices of (a) and (d) are identical in Fourier space (b) and (e). This feature can be utilized for the detection of scanning probe artifacts.

Keywords: crystallographic image processing, scanning probe microscopy, scanning tunneling microscopy