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Progress in Crystallographic Image Processing for Scanning Probe Microscopy

Peter Moeck and Jack Straton

Nano-Crystallography Group, Department of Physics, Portland State University, Portland, OR 97207-0751

Crystallographic Image Processing (CIP) originated with the electron crystallography community. Nobel Laureate Sir Aaron Klug (OM, FRS) and coworkers pioneered the technique for the analysis of long-range ordered biological materials in parallel illumination Transmission Electron Microscopes (TEMs). Corrections for the effects of the TEM's phase contrast transfer function and for less than optimal imaging conditions are part of this kind of CIP. There are also "electron microscope independent" 2D crystallography foundations to this kind of image processing.

Based on these foundations, we applied CIP to images of long-range ordered 2D periodic surface arrays that were recorded with different kinds of scanning probe microscopes (SPMs) [1,2]. We amended our method recently [3] to detect and correct frequently encountered artifacts in scanning probe microscopy, i.e. effects of multiple mini-tips that collectively result in a blunt tip [4,5]. Loosely speaking, our version of CIP has the effect of "sharpening up" a blunt scanning probe tip. This is achieved by the deconvolution of the prevailing microscope's point spread function from the SPM images. Although many scanning probe microscopists have so far been content with ignoring these kinds of artifacts, there are also highly credible reports on unambiguous observations on scanning probe tip changes during data recordings that led to blunt tip artifacts in SPM images [6,7]. One of these reports proposes that multiple mini-tips cannot affect the character of the observed translation symmetry in such an image while the 2D periodic motif may be smeared out [6].

Our theoretical analysis [4] confirms this idea so that one can confidently take "inconsistencies" between observed 2D translation and point symmetries in SPM images (Fig. 1) as the hallmark of multiple mini-tip artifacts. Our unambiguous determination of the underlying Bravais lattices of 2D periodic surface arrays [3] on the basis of a geometric Akaike Information Criterion (AIC) [8] achieves the detection of multiple mini-tip artifacts on a statistically sound basis. Figure 1 demonstrates the effectiveness of our version of CIP in removing blunt tip artifacts from a simulated scanning tunneling microscope (STM) image of long-range ordered 2D periodic arrays of cobalt-phthalocyanine molecules on a (001) oriented gold surface. Note that the central circular area in the left part of Fig. 1 illustrates both (*i*) an inconsistency between 2D translation and point symmetries and (*ii*) the fact that structural scanning probe tip changes during the recording of experimental data cannot change the character of the observed translation symmetry in the resulting SPM image.

Our recently developed unambiguous translation symmetry determination procedure [3] also constitutes progress towards making CIP more objective in both electron crystallography by TEM and surface feature assessments by SPM. This is because not all plane symmetry groups are disjoint. As it is well known, all of the symmetry operations of a plane symmetry group are contained in its so called *translationengleiche* minimal supergroup [9]. The application of the traditional quantifiers of the deviations of experimental images from their plane symmetry enforced counterparts (as used in electron crystallography) can, therefore, never be completely objective [1,4]. Because the practitioners of electron crystallography have typically chemical intuition (and sometimes prior knowledge) about the atomic arrangement they are trying to solve and often work with multiple 2D projections of the same 3D crystals, this lack of complete objectivity is tolerable in that field. Scanning probe microscopists that are trying to utilize CIP in their field are less fortunate as they need to work from one 2D projection only. Geometric AICs [8] have specifically been developed to select the best model out of a set of non non-disjoint models so that their application in CIP for

SPM is mandatory. Associated with the usage of geometric AICs in CIP [4,5] is, however, the requirement that systematic errors in 2D periodic images need to be corrected to such a level that they become small compared to random errors [10].

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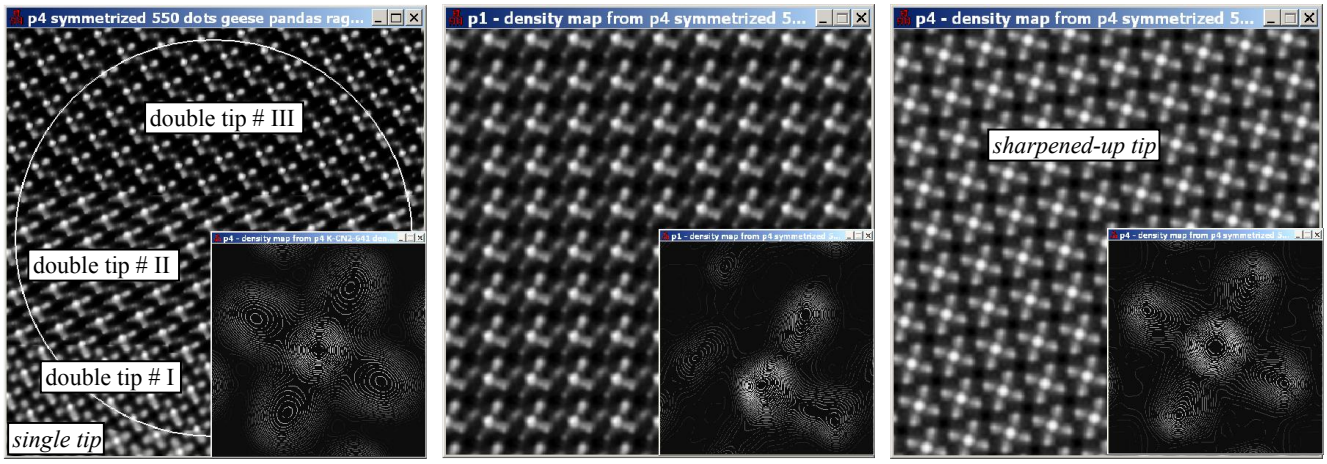

Figure 1. Demonstration of the CIP removal of double-tip artifacts in scanning probe microscopy. **Left:** simulated raw data. The very small stripe at the bottom of this image represents the sample as imaged with a single scanning probe tip. The three wider stripes represent the sample as imaged with double tips of different geometries. The inset represents 1.1 unit cells of the sample array as imaged with a single tip as contour plot with 32 gray scale levels. **Middle:** Classical Fourier filtering of the image (to the left) cannot remove double (and multiple) scanning probe mini-tip artifacts as it represents only translation symmetry averaging. **Right:** CIP result on the circled area in the raw data (i.e. the first image in the row). The insets in the last two images of this row represent 1.1 unit cells of the middle and right array as contour plots with 32 gray scale levels. Note the striking similarity of the left and right inset, which demonstrates the above mentioned sharpening-up of the scanning probe tip. The 2D periodic motif in all three insets is approximately 1.5 nm wide. Note also that 2D periodic motifs with point symmetry *1* (i.e. no other point symmetry than a rotation by 360°) in the first two images in this row are inconsistent with the clearly recognizable square Bravais lattice, because that kind of 2D translation symmetry requires as part of the plane symmetry groups *p4*, *p4mm*, and *p4gm* two Wyckoff positions that posses at least point symmetry *4*.