Crystallographic image processing for scanning probe microscopy

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Crystallographic image processing (CIP) is a set of techniques that allow for the extraction of crystallographic information [1] and also for the “improvement” of experimental images of 2D-periodic objects. CIP works on the basis of the determination and enforcement of plane symmetries. An experimental image may contain defects, distortions and other imperfections that are partially due to the real object and partially caused by the imaging device. If the real object consists of a large and regular array of 2D periodically arranged motifs that have nearly the same internal structure, CIP will remove random distortions by averaging a raw image over all motifs. Mathematically, an experimental image is the convolution of the object with the point spread function of the microscope (PSF). Thus, the reconstruction of the true object structure can be done by deconvoluting the PSF from the experimental image. Assuming that the PSF contains all information about aberrations and imperfections of the imaging device, the deconvolution of the experimental image yields an “aberration free” image of the object. Typically, the PSF is unknown and, hence, its extraction requires special efforts. One extraction strategy is to image a known (reference) object. The PSF is then used for the deconvolution of images from unknowns. Another strategy is referred to as “symmetrization”, in which we directly exploit the 2D-periodic (and symmetric) nature of the raw image, e.g. Fig. 1a. The method utilizes then the relations between symmetry related Fourier coefficients of the image intensity, which allow for an effective point symmetry averaging over the periodic motif, Fig. 1b. The resulting PSF is shown in Fig. 1c.

Here we present dedicated PC software for the crystallographic processing of “any 2D periodic array of features”. Some modifications to the algorithms of ref. [1] were introduced in order to boost the performance of our program. Our stand-alone program consists of two independent modules: 1) the image-processing module, Fig. 2a, which performs the Fourier analysis of a raw image, auto correlation, and peak search; and 2) the symmetrizing module, Fig. 2b, which performs symmetrization in accordance with the algorithms of ref. [1]. These two modules applied consecutively lead to the creation of two-dimensional images with enforced plane symmetry, as required by the mathematical restrictions imposed by a user-selected plane group. As “figures of merit” of the results of symmetrizing using different plane groups, the Fourier coefficient residuals can be used. There are two types of residuals: amplitude residuals:

$$F_{res} = \frac{\sum |F_{hk}^{obs} - F_{hk}^{sym}|}{\sum |F_{hk}^{obs}|},$$

and phase residuals:

$$\alpha_{res} = \frac{\sum F_{hk}^{sym} \cdot |\alpha_{hk}^{obs} - \alpha_{hk}^{sym}|}{\sum F_{hk}^{sym}},$$

see Fig. 2b.

They measure the deviation of the Fourier amplitudes and phases of the symmetrized image intensity ($\alpha_{hk}^{sym}$, $F_{hk}^{sym}$) from their counterparts of the raw image ($\alpha_{hk}^{obs}$, $F_{hk}^{obs}$). The smaller the residuals (especially the phase residual), the better is the symmetrized image an “improved” version of the raw image. If systematic errors are well corrected for, lower residuals also indicate more truthful representations of the averaged 2D-periodic motif of the sample.

We also tested the idea of using cross-correlations between raw STM images and symmetrized images in conjunction with the CIP procedures in order to come to more objectively quantifiable
decisions on the most likely plane symmetry that an experimental image possesses. The height of the central peak in cross-correlation maps, i.e. $CCF(0,0)$ as calculated by the relation below, may indeed be used as a quantitative measure of the similarity of the symmetrized and the raw image. For the raw image of Fig. 1a symmetrized to the plane group $p31m$ (by the program of ref. [1]), we obtained the maximal value (i.e. $3.254 \times 10^8$) of the $CCF(0,0)$ for all hexagonal groups and a reasonably low phase residual (i.e. $26.2^\circ$). This suggests both that this is the correct plane symmetry and that the mirror lines in isolated HAT(CN)$_6$ molecules are broken when they become part of a 2D-periodic regular monolayer array on Ag (001). The cross correlations were calculated using the relation:

$$CCF(x,y) = \frac{\sum \sum [i(x',y') - \langle i(x',y') \rangle] \cdot [t(x' - x, y' - y) - \langle t \rangle]}{\sqrt{\sum \sum [i(x',y') - \langle i(x',y') \rangle]^2 \cdot \sum \sum [t(x' - x, y' - y) - \langle t \rangle]^2}},$$

where $x$ varies from 0 to $x_{\text{max}}$, $y$ varies from 0 to $y_{\text{max}}$, $i(x,y)$ represents the symmetrized image; $t(x,y)$ represents the template; $\langle \cdot \rangle$ is the average value of the pixels in $i(x,y)$; $\langle i(x',y') \rangle$ is the average of $i(x,y)$ in the region covered by the current location of $t$.

References


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