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Noise Removal by Crystallographic Averaging and Information Content of an Image With Respect to Detections of Plane Symmetries

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Crystallographic Image Processing (CIP) allows for the extraction of good estimates of the phases of the structure factors of many inorganic crystalline materials when the conditions of the (pseudo) weak phase object approximation are met in parallel-illumination high-resolution transmission electron microscopy (TEM) [1]. In atomic-resolution scanning TEM, CIP has been employed to remove noise from images and to confirm the average alkali-metal content per unit cell in a type I silicon clathrate [2]. The CIP technique has also been utilized to improve the signal to noise ratio (S/N) of scanning probe microscopy (SPM) images, reveal individual molecules more clearly [3,4], and remove the effects of multiple scanning probe mini-tips on a blunt scanning tunneling microscope (STM) tip from the images [5]. Because spatial averaging in CIP is done over all "asymmetric fraction" of all unit cells of regular 2D periodic arrays, this kind of noise removal from 2D periodic images is up to twelve times more effective [3,4] than traditional Fourier filtering [6].

The effectiveness of crystallographic averaging by CIP is demonstrated in Figure 1 on noisy images that were created with the popular freeware program GIMP on the basis of STM data that were published in ref. [7]. The first column of this figure shows the effect of traditional Fourier filtering (*p1* enforcing) on images with from top to bottom progressively worsening S/Ns. The second and third columns show the effects of crystallographic averagings in Fourier space that take plane symmetries *p2* ("extra averaging factor" of 2 gained) and *p4* ("extra averaging factor" of 4 gained) into account. The program CRISP [1] was used for these purposes and also for the determination of the entries in the table to the right of Fig. 1.

The conclusion on the most probable* plane symmetry (*p4*) that underlies this STM data [7] was reached on the basis of the application of our geometric Akaike information criterion (G-AIC) to the detection of the underlying 2D translation lattice [4]. These kinds of criteria are only applicable when there are negligible systematic errors [8], which should be the case for experiments with well calibrated modern STMs and TEMs. Traditional plane symmetry deviation quantifiers for symmorphic 2D space groups are the residuals of the Fourier coefficient amplitude (A_{res}) and phase (φ_{res}) [1,3,4] as listed in the table to the right of Fig. 1 for the (not shown) test images that underlie this demonstration. Note the increase of the difference between the phase residuals for *p2* and *p4* with reduced S/Ns. The square root of the ratio of two G-AIC values (that were calculated on the basis of squared plane symmetry deviation quantifiers) can be utilized as a measure of the noise dependent information content [8] of a STM, SPM, TEM, or scanning TEM image with respect to the detection of the underlying plane symmetry of the regular periodic array from which it was recorded [9].

The raw STM image [7] that served as foundation of Fig. 1 was run through a low-pass (Gaussian blur) filter before Gaussian noise was added in a systematic way. The insets in each row are histograms of the (not shown) gray-level test images that resulted from this addition of Gaussian noise to the same (not shown filtered) STM image. The table gives traditional plane symmetry deviation quantifiers [1,3,4] for these (not shown) images for selected plane symmetry groups and the average of all subgroups of *p4mm* other that *p4* and *p2*. It is clear from the histograms and the table that the S/N gets progressively worse from top to bottom.

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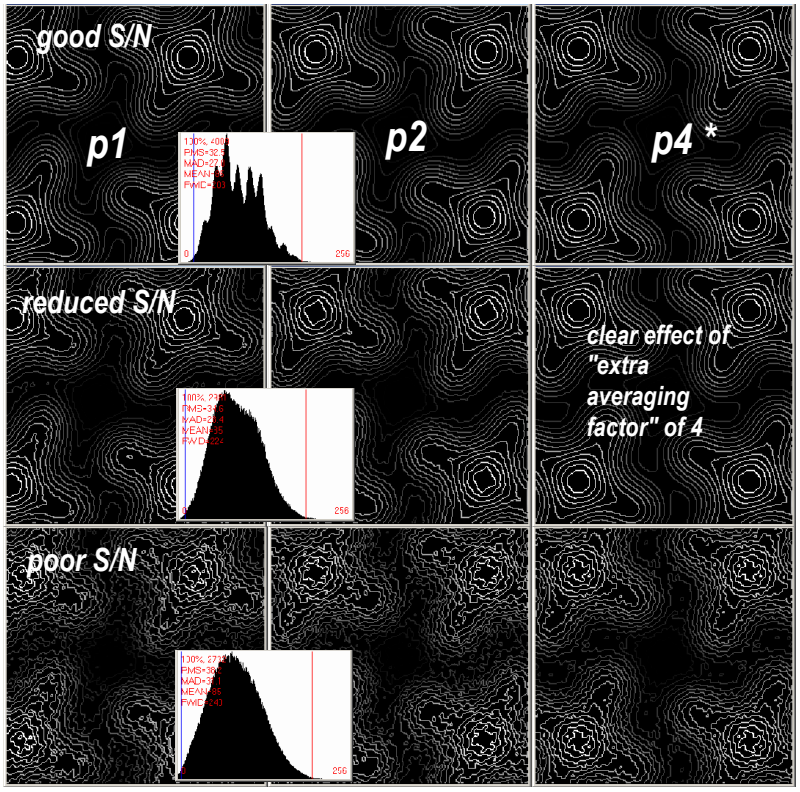

Good signal to noise ratio (S/N), only one "Gaussian noise unit" added	A_{res} **in %**	φ_{res} **in °**
p2 (n.d. means not defined)	n.d.	5.3
p4	8.6	5.3
average of all other subgroups of p4mm	13.3	12.1
p4mm	18.9	19.3
Reduced S/N, three times more Gaussian noise added (loosely speaking)	A_{res} **in %**	φ_{res} **in °**
p2	n.d.	8.4
p4	10.9	8.4
average of all other subgroups of p4mm	16.6	13.0
p4mm	22.2	21.5
Poor S/N, five times more Gaussian noise added (loosely speaking)	A_{res} **in %**	φ_{res} **in °**
p2	n.d.	17.3
p4	18.7	18.7
average of all other subgroups of p4mm	23.1	18.7
p4mm	31.8	30.7

Figure 1. Averaging over approximately forty cobalt(II)phthalocyanine ($C_{32}H_{16}CoN_8$, each approx. 1.4 nm across) molecules in a regular 2D periodic array on gold (111). **First column:** translation only (*p1*) averaging; **second column:** *p2* enforced averaging; **third column:** *p4* enforced averaging. ***Progressively more Gaussian noise has been added from top to bottom*** for the sake of this demonstration, so that the signal to noise ratio (S/N) gets progressively worse. The "tetra-lobe features" in the (not shown) original STM image [7] are direct space representations of the local electronic density of states of the molecules at the Fermi level and their "fine scale appearances" in contour level maps depend on the sample bias, noise, and a range of experimental parameters.
***** Since the 2D lattice vectors were determined to differ by only 2.7 % in length and intersect at an angle of 90.8° [4], it is possible that the $C_{32}H_{16}CoN_8$ molecules in their 2D periodic array [7] possess only (2D) point symmetry *2* within an oblique 2D Bravais lattice that is pseudosymmetric (http://reference.iucr.org/dictionary/Pseudo_symmetry) to a square lattice (when projected orthogonally from 3D).

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