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Crystallographic symmetry classifications of noisy 2D periodic images in the presence of pseudo-symmetries of the Fedorov type

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Crystallographic symmetry classifications (CSCs) are a crucial part of the crystallographic processing of noisy 2D periodic images from crystals and crystal surfaces. Based on these classifications, the images can subsequently be corrected for having been recorded under suboptimal imaging conditions. For images that have been recorded within the weak-phase-object approximation of transmission electron microscopy, these corrections allow for the extraction of good estimates of the phase angles of the projected structure factors [1]. Good estimates of these phase angles are crucial for the solving of crystal structures by means of electron crystallography [1]. In case of scanning probe microscopy, crystallographic image processing allows for the correction of the effects of a blunt scanning probe tip [2,3]. Severe problems in the CSC of more or less 2D periodic images may arise from the co-existence of a large amount of imaging noise and pseudo-symmetries of the Fedorov type [4]. Pseudo-symmetries of that particular type are compatible with a Bravais lattice that does not necessarily need to be the prevailing Bravais lattice of the hypothetical noise-free version of the image. In noisy 2D periodic images, these kinds of pseudo-symmetries are, therefore, difficult to distinguish from the genuine symmetries of that hypothetical image so that mis-classifications may result.

Traditional electron crystallography utilizes three complementing plane symmetry deviation quantifiers [1,2] for its CSC procedures. Two of these quantifiers are (dimensionless) ratios. The third and most valuable traditional plane symmetry deviation quantifier of traditional electron crystallography is the average difference of the phase angles of the raw and symmetrized Fourier coefficients of 2D periodic images. None of these three quantifiers is, however, in a form that allows one to use them as parts of geometric Akaike Information Criteria [5]. As a result of this, they need to be evaluated by a researcher on the basis of a set of rules [1] which are of a more or less qualitative (rather than fully quantitative) nature. Traditionally performed CSCs are, therefore, always *subjective* in spite of the best efforts of the researchers. Pseudo-symmetries of the Fedorov type in a noise-free and strictly 2D periodic image with plane symmetry group *p1m1*, Figs. 1a and 2, combine (for demonstration purposes) with generalized imaging noise, Figs. 1b,c, to more or less 2D periodic images that "apparently" possesses a pseudo-square lattice and plane pseudo-symmetry group $p_{b/3}4mm$ or one of its subgroups/superlattices. Note that *p1m1* is one of these subgroups, but is based on a rectangular Bravais lattice, which is an "apparent" superlattice. The correct unit cell is three times larger than the pseudo-square translation cell. Two different computer programs that are dedicated to electron microscopy and crystallography [1] were in their default settings unable to extract lattice parameter information from the noisy images in Figs. 1b,c that would allow for their correct CSCs into the rectangular Bravais lattice type [6]. This was due to the weak 0,1 Fourier coefficients (FCs) that these programs ignored. Both programs took the 0,3 FCs instead as end points of $\vec{b}*$, which are then equal in magnitude to $\vec{a}*$.

Following an information theory based approach that utilizes geometric Akaike Information Criteria [5], symmetry information content measures [7], confidence levels [7], as well as Akaike weights and their products [8], the CSC rules of traditional electron crystallography [1] and the inherent subjectivity in applying them are replaced by numerically derived inequalities that are either fulfilled or not, allowing for completely objective determinations. Information that allows for subsequent classification into Bravais lattice types [7,8], Laue classes [8], and plane symmetry groups [8] can be straightforwardly extracted from noisy 2D periodic images. Such information can be combined into suitable Akaike weight products (i.e. updated Bayesian posterior model probabilities [8]) when one encounters strong pseudo-symmetries of the Fedorov type and/or when the images are very noisy.

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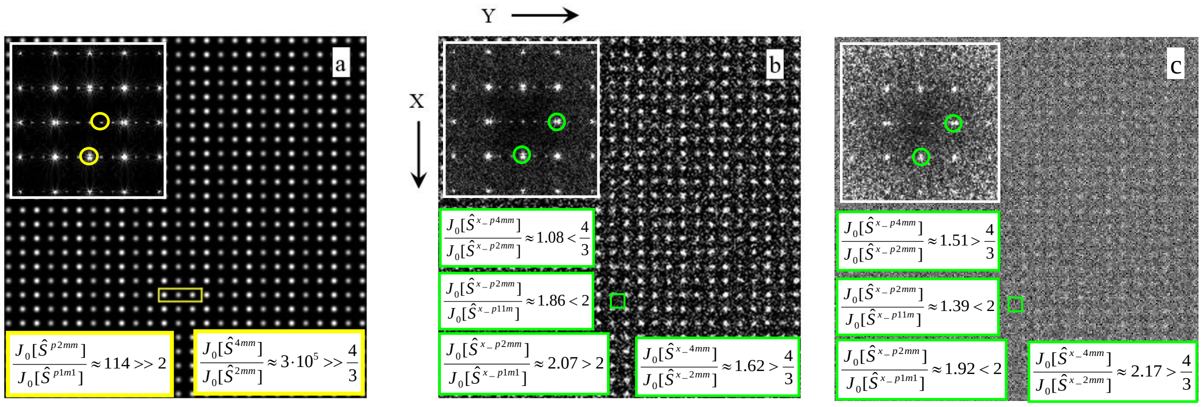

Figure 1. Illustration of the combined effects of Fedorov pseudo-symmetry and Gaussian noise. **(a)** Noise-free and strictly 2D periodic image with plane symmetry group *p1m1* and a rectangular Bravais lattice that possesses an *a*/*b* ratio of one third. **(b)** The image in (a) with independent Gaussian noise of mean zero and a standard deviation of 10 % of the maximal image intensity added. **(c)** The image in (a) with the same type of noise but a five times larger standard deviation added. The insets in all three images are the amplitude maps of the discrete Fourier transforms (dFTs) of the maximal circular areas that each image permits one to select, the CSC defining inequalities, and a "perceived" unit cell outline. The circled spots in the dFTs in (b) and (c) define pseudo-translation lattices in Fourier space. On the basis of these lattices, the Kullback-Leibler best plane symmetry groups are identified in (b) correctly as $p_{b/3}1m1$ and in (c) incorrectly as $p_{b/3}2mm$ (which is a minimal supergroup of the correct group as well as a minimal subgroup of pseudo-symmetry group $p_{b/3}4mm$). Note that all very weak FCs of the images in (b) and (c) did not contribute to the numerical values of their CSC defining inequalities. When we allow for their contributions (by choosing the correct lattice manually – results not shown here), the correct plane symmetry groups are unambiguously identified by our new information theory based CSC method [8] in both cases. We, thus, developed a method that deals effectively with Fedorov pseudo-symmetries [4] in the presence of relatively high levels of generalized imaging noise.

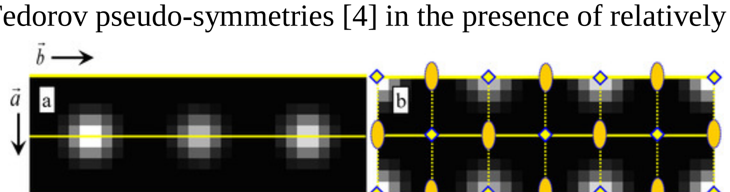

Figure 2. Demonstration of genuine and pseudo-symmetries in Fig. 1a, reproduced from [8]. **(a)** Three parallel mirror lines are the genuine symmetries of plane symmetry group *p1m1* as shown within a unit cell. **(b)** The mirror lines of (a) for an alternative origin choice of *p1m1* combine apparently with pseudo-symmetries of the Fedorov type to plane pseudo-symmetry group $p_{b/3}4mm$ and its subgroups/superlattices.

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