Crystallographic Image Processing for Scanning Probe Microscopes

T. Bilyeu, B. Moon Jr., P. Moeck

Portland State University, Department of Physics. PO Box 751, Portland, Oregon 97207 USA

The crystallographic processing of two-dimensional (2D) periodic transmission electron microscopy (TEM) images of inorganic crystals was first demonstrated by Sir Aaron Klug over 30 years ago [1]. Since that time crystallographic image processing (CIP), as it has become known, has been used in the electron crystallography community to aid in the determination of three-dimensional crystal structures based on high-resolution TEM images. More recently, we have shown that CIP can be used to process scanning tunneling and atomic force microscope images [2,3]. We are currently developing a dedicated CIP computer program for the Scanning Probe Microscopy (SPM) community.

The 17 crystallographic plane symmetry groups [4] are models for 2D periodic images. Hence any SPM image of a regular 2D array of molecules aligned on some surface should belong to one of these 17 plane groups if imperfections in the imaging process were corrected for. A set of symmetrized Fourier coefficients can be calculated for each plane symmetry group by imposing their symmetry relations on the experimental Fourier coefficients. The decision on which plane symmetry group is most likely present in the experimental image has traditionally been made based on some combination of prior knowledge and calculated residuals which quantify how much the experimental Fourier coefficients deviate from each set of symm etrized Fourier coefficients. In addition to this, our program uses a geometric Akaike information criterion (GAIC) to narrow down the number of probable groups to 5 or less, based on the shape of the unit cell. Traditional CIP residuals can then be used to discriminate between this smaller subset of groups.

Our program, preliminarily titled T4SC (Tools for SPM based CIP), consists of several main modules (two of which are partially shown in Figure 1): a lattice detection module, an image symmetrization module and a point spread function (PSF) module. In the lattice detection module, a Fast Fourier Transform is performed on a user selected area of an experimental SPM image, resulting in a set of (complex) Fourier coefficients. This gives two parallel sets of data: an amplitude map and a phase map. A peak-search procedure is employed to filter out erroneous peaks in the amplitude map. Once this is accomplished, the valid peaks are used to index the amplitude part of the Fourier transform and determine the shape of the unit cell, as well as the 2D lattice present.

The image symmetrization module is responsible for calculating the symmetrized Fourier coefficients for each plane symmetry group. Additionally, traditional CIP residuals and GAIC coefficients are calculated and a decision is made about which plane symmetry group is to be enforced. Finally, an inverse Fourier transform is performed to output the CIP corrected image.

The PSF module allows for the calibration of a SPM based on the CIP results. An experimental image is just the convolution of an object and the PSF. In reciprocal space, the convolution integral becomes a simple multiplication. If we then divide the experimental image by the CIP corrected image of a highly symmetric calibration sample (which we treat as the object), the result is the Fourier transform of the PSF. The PSF is extracted within the PSF module following the above
concepts. Subsequent images taken on the same microscope with the same tip under approximately the same experimental conditions can then be corrected by the same PSF. This is especially useful if the user lacks prior knowledge about the plane symmetry in the sample and the image symmetrization module is unable to determine the most likely symmetry with the desired certainty.

We show that the GAIC is successful in determining the most likely plane symmetry group present in real experimental SPM images, when compared to decisions based on traditional CIP residuals alone. We also demonstrate the successful extraction of the PSF for an SPM by carrying out the CIP procedure on a calibration sample. Work is currently being done to develop a more general GAIC which uses pixel intensity variations throughout the entire unit cell rather than just its shape. This would allow us to discriminate between the 17 plane groups directly.

References:

[1] Klug, A., “Image Analysis and Reconstruction in the Electron Microscopy of Biological Macromolecules,” Chemica Scripta 14, 245-256 (1979).

[2] Moeck, P., “Crystallographic image processing for scanning probe microscopy,” In Microscopy: Science Technology, Applications and Education, Microscopy Book Series, vol. 3 (no. 4), pp. 1951–1962, A. Méndez-Vilas and J. Díaz (editors), Formatex Research Center, 2010; http://www.formatex.info/microscopy4/1951-1962.pdf

[3] Moon, B. Jr., “Employment of crystallographic image processing techniques to scanning probe microscopy images of two-dimensional periodic objects,” MSc thesis, Portland State University, Dept. of Physics, 2011, http://nanocrystallography.research.pdx.edu/papers/thesis14acorr.pdf

[4] Hahn, T., Editor, International Tables for Crystallography Volume A: Brief Teaching Edition, 5th ed., Dordrecht, The Netherlands, Wiley, 2005.

[5] Portland State University’s (PSU’s) support in the form of Faculty Enhancement, Internationalization, and Research Stimulus Awards is gratefully acknowledged. PSU’s Venture Fund also supported this project.

FIG. 1. Screenshots showing portions of the lattice detection module (left) and the image symmetrization module (right). A simulated image with $p4mm$ symmetry was used for these examples. Approximately $\frac{1}{4}$ of the indexed Fourier amplitude map is shown in the lattice detection module. Residuals typically used to decide which plane symmetry group should be enforced on an experimental image are shown in the image symmetrization module.