Fast periodicity-analysis with “4spots” and ImageJ

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Scattering experiments in the transmission electron microscope (TEM) result in a large number of phase-identification challenges. This note is first in a series on the inverse-problems associated with Bayesian model-selection and parameter-estimation [1] from TEM data. In particular here we present a fast method for determining two g-vectors and an inter-spot angle from **your** diffraction and HREM images.

Ways to analyze that data for candidate-structure elimination, indexing & orientation-determination of recognized-structures [2], and (with data taken at more than one tilt) direct 3D lattice-parameter determination [3] are discussed elsewhere, as are ways to simulate such data from candidate structures [4], [5]. Our method is easily portable, using the freely available image-processing software ImageJ. Plugins and follow-on routines will also be made available freely on the web [6].

In the case of single crystal SAED data, the essential problem is the determination of two g-vectors along with the angle between them. By choosing two pairs of symmetric reciprocal lattice points around the un-scattered beam, one can compute the equations of two lines containing each pair of points. The intersection point of the two lines can then be used in conjunction with one point from each pair to determine g-vectors for each of the two point pairs. The dot product of the two g-vectors can now be used to determine the angle between the two g-vectors. With knowledge of camera constant, the d-spacings associated with each of the g-vectors can be computed. When the camera constant is not known, one may still make use of the ratio of g-vectors to begin the identification of candidate structure. Our straightforward treatment of the problem allows one to rapidly obtain two d-spacings and an inter-spot angle for any SAED data point having two pairs of symmetric reciprocal lattice points. Our imageJ plugin, “4spots”, performs these computations and outputs g-vectors, d-spacings, and inter-spot angle.

In a similar fashion, the analysis of HREM data may be reduced to one of simple point selection about an un-scattered beam. To obtain a set of symmetric points, one first will need to use the FFT feature built in to imageJ. We begin by selecting a suitably sized square, cropped from a region of HREM data that exhibits lattice fringes. We find that 1024 × 1024 pixel regions are generally most suitable due to typical memory limitations. The FFT of such a square is then computed, resulting in an equal sized image with points located at positions determined by periodicities present in the HREM data. One can now analyze the data in a manner analogous to SAED data, using our “4spots” plugin to choose two pairs of symmetric spots and obtain g-vectors, d-spacings, and an inter-spot angle. Follow-on routines e.g. to rule out or to explore plausible indexings with candidate lattices will be discussed as well [7].

References:

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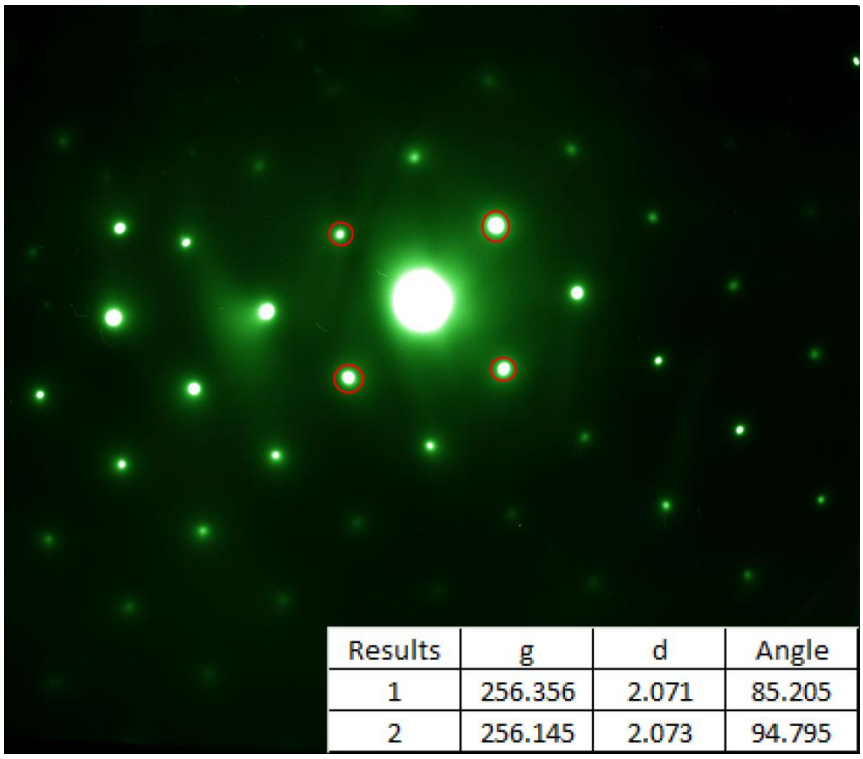

Results	g	d	Angle
1	256.356	2.071	85.205
2	256.145	2.073	94.795

Typical SAED diffraction data obtained from a possible ZrC inclusion in ZrB_2 ceramic. The inset table shows the results of our 4spots plugin run using the points circled in red. The indicated results rule out the possibility of ZrC, but suggest the presence of an unexpected phase B_4C.