MS2-O5 Phase retrieval for randomly terminated finite crystals

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In serial femtosecond nanocrystallography with x-ray free-electron lasers, diffraction data can be obtained from crystals that have a small number of unit cells [1]. The fewer number of unit cells means that the diffraction patterns from these nanocrystals contain measurable information between the Bragg reflections courtesy of a lattice/shape transform that is no longer delta-like.

By separating the effect of the shape transform from the diffraction via its inherent periodicity about the reciprocal lattice [2], the averaged diffracted intensity from all crystals can be directly converted into the diffracted intensity of a single unit cell. The problem then becomes that of reconstructing a single, non-periodic object (the contents of the unit cell) from the amplitude of its Fourier transform, which is known to have a unique solution that can be found using iterative phase retrieval algorithms [3,4].

However, if there is more than one molecule per unit cell then the inter-Bragg diffraction from such crystals will depend on the particular configuration of the molecules on the crystal surface, as different unit cells can be defined for different surface terminations. To a first approximation, the diffraction of the unit cell recovered from the method described above is no longer that of a single kind of unit cell but is equal to the incoherent average over a set of unit cells that contain different arrangements of the molecule based on the space group at hand [5,6].

Following from the recent experimental success of shape transform phasing of synthetic crystals without randomly terminated edges [7], the applicability of direct iterative phase retrieval when multiple unit cells are present is explored using experimental data collected from synthetic crystals with random edge terminations at the FERMI free-electron laser in Trieste, Italy. Results so-far indicate successful phase retrieval under this circumstance is still possible.

References

[1] H.N. Chapman *et al.*, *Nature*, **470**, 73-78 (2011).

[2] J.C.H. Spence *et al.*, *Opt. Express*, **19**, 2866-2873 (2011).

[3] R.P. Millane, *J. Opt. Soc. Am. A*, **7**, 394-411 (1990).

[4] S. Marchesini, *Rev. Sci. Instrum.*, **78**, 011301 (2007).

[5] J.P.J. Chen and R.P. Millane, *J. Opt. Soc. Am. A*, **31**, 1730-1737 (2014).

[6] R.A. Kirian *et al.*, *Phil. Trans. R. Soc. B*, **369**, 20130331 (2014).

[7] R.A. Kirian *et al.*, *Phys. Rev. X*, **5**, 011015 (2015).

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