

MS09-02 | MASK-BASED APPROACH TO RESTORING AND PHASING SINGLE-PARTICLE DIFFRACTION DATA

Lunin, Vladimir (Keldysh Institute of Applied Mathematics, Pushchino, RUS)

The development of experimental techniques, in particular the emergence of the X-ray free-electron lasers, allows to approach the practical solution of the problem of registration of the scattering from an isolated particle and thereby to obtain information about the three-dimensional structure of non-crystalline biological objects by X-ray diffraction methods. The possibility to measure non-Bragg reflections makes experimental data mutually dependent and essentially simplifies the structure solution. Sampling of experimental scattering data to a fine enough grid makes the structure determination equivalent to phasing of structure factor magnitudes for an 'imaginary' crystal with extremely large solvent content. This makes density modification phasing methods especially powerful supposing the object envelope is known. At the same time, such methods may be sensitive to the accuracy of the envelope and completeness of experimental data and may suffer from nonuniqueness of the phase problem solution. The mask based approach is a preliminary phasing method that performs random search for connected object envelopes that produce the estimates of structure factor magnitudes close to the values observed in X-ray experiment. Alignment, clusterization, and averaging of the phase sets corresponding to selected putative envelopes produce an approximate solution of the phase problem [1,2]. Beside the estimating of unknown phase values this approach allows to estimate the values of structure factor magnitudes lost in the experiment, *e.g.* ones corresponding to beam-stop shade zone or to oversaturated reflections.

[1] Lunin et al.: Acta Cryst. D72, 147-157

[2] Acta Cryst. D75, 79-89