Image reconstruction from diffraction patterns in coherent X-ray diffraction imaging using the dark-field phase-retrieval method

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In coherent X-ray diffraction imaging (CXDI) experiment, we reconstruct the electron density map of specimen particle, which is projected along the direction of incident X-ray, using the iterative phase-retrieval (iPR) method. We have developed a program suite [1,2], in which the iPR algorithm is implemented together with miscellaneous subroutines, and applied to simulation studies on the possibility of molecular imaging using X-ray free electron laser [1,2] and structure analysis for experimentally obtained diffraction patterns of chloroplasts [3]. One of problems in CXDI experiment is the difficulty to collect diffraction patterns of very small-angle region, where the information regarding particle shape is included.

Recently, the dark-field phase-retrieval (DFPR) method [4] is applied to diffraction patterns lacking the diffraction patterns of small-angle region, and demonstrated the possibility to give shape information. In the method, a monotonously decreasing mask function is multiplied to high angle diffraction pattern prior to conduct ordinary iPR calculation. After that, the ordinal iPR method is applied.

In the present study, we implemented the DFPR algorithm to our iPR program suite and examined carefully the effectiveness of the methods through a series of phase-retrieval simulations regarding a protein molecule. Even when lacking a large area around the incident beam up to the 5-th speckle patterns counted from the incident beam, the shape of the protein molecule is correctly reconstructed. Subsequent iPR calculation using the density map obtained by the DFPR method successfully retrieved the projection molecular image. In this poster session, we report the details of the DFPR method and future application.

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