High-Spatial-Resolution X-ray Diffraction Microscopy

Yoshinori Nishino, Yukio Takahashi, and Tetsuya Ishikawa

SPring-8/RIKEN, 1-1-1 Kouto, Sayo-gun, Sayo-cho, Hyogo, 679-5148 Japan

X-ray diffraction microscopy is a novel method to reconstruct electron density distribution from the x-ray diffraction intensity data with no need of sample crystallization. In experiment, the x-ray diffraction intensity pattern is measured at fine intervals in the reciprocal space to satisfy the oversampling condition for solving the phase problem. The phase set is recovered from the oversampled diffraction intensity data by applying an iterative method by Gerchberg, Saxton, and Fienup. Short wavelength and high penetration power of the x-ray offer the unique possibility to achieve high-spatial-resolution three-dimensional structural analysis for non-crystalline samples.

The spatial resolution s in x-ray diffraction microscopy, as in other diffraction-based methods, is inversely proportional to the maximum size of the scattering vector $\boldsymbol{K}$, and is given by $s = 2\pi/\max(|\boldsymbol{K}|)$. Here, the size of the scattering vector is defined as $|\boldsymbol{K}| = 4\pi \sin(\Theta/2)/\lambda$, and λ and Θ are the x-ray wavelength and the scattering angle, respectively. From the mathematical expressions above, it is clear that shorter wavelength x-rays and wider aperture detector system are beneficial to gaining higher spatial resolution. In our diffraction microscopy experiments at SPring-8, short-wavelength hard-x-rays have been used for the purpose. In addition, we are developing a large-area in-vacuum imaging plate detector for further improvement of spatial resolution [1].

According to Porod's law, the diffraction intensity scales as $|\boldsymbol{K}|^{-4}$ for large $|\boldsymbol{K}|$, and therefore the radiation dose required to achieve a certain spatial resolution s grows as s^{-4}. Because the increase of the radiation dose may cause sample damages, especially for biological samples, radiation damage may set the limit of the highest spatial resolution.

As a way to circumvent the radiation damage problem, we discuss a possibility of achieving super-resolution in data analysis. Here the super-resolution implies to retrieve diffraction amplitudes (moduli and phases) at higher $|\boldsymbol{K}|$ than actually measured. Pioneering works in this respect is due to Gerchberg and Papoulis in mid 1970's. Some results of super-resolution in simulation and in experimental data analysis will be shown.

[1] Y. Nishino, J. Miao, Y. Kohmura, Y. Takahashi, C. Song, B. Johnson, M. Yamamoto, K. Koike, T. Ebisuzaki, and T. Ishikawa: Proceedings of the 8th International Conference on X-ray Microscopy (The Institute of Pure and Applied Physics, Tokyo, 2006) in press.