Poster Presentation

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SHIKA: a fast and accurate spot finder for raster scan on microfocus beamlines

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On BL32XU, a microfocus beamline at SPring-8, oscillation data are collected with typical horizontal beam size of 1 μm. Hence it requires very accurate crystal centering, which is difficult especially for invisible crystals e.g. LCP crystals. Therefore, we perform raster diffraction scan to find crystal positions based on their diffractivity using low-dose exposure. It had been time consuming process due to two reasons; i) slow readout time of CCD, ii) manual inspection of hundreds of diffraction images. To tackle this problem, we installed new fast-readout CCD detector, MX225HS (Rayonix, L.L.C.), and developed support tool for raster scan based crystal centering. The tool visually shows possible crystal position on 2D map based on spot populations, and therefore it is named SHIKA (Spot-wo Hirotte Ichiwo Kimeru Application; a Japanese abbreviation which means the application for crystal positioning by picking up spots). SHIKA automatically detects new images when raster scan started and finishes just after raster scan ends. On GUI, user can find and pass the crystal position information to KUMA (a tool suggesting helical data collection strategy with predicted radiation damage) to start data collection immediately. User can also see picked spots on diffraction images with GUI. SHIKA has been developed based on DISTL [1] and modified to be faster and more accurate, especially for LCP crystal which is an important target on BL32XU. SHIKA picks up spots after subtracting smoothed pseudo-background which is a key for better separation of spots and ring-like diffuse background of lipids. Smoothing is time-consuming, but SHIKA now uses GPUs for almost all process including high-speed median filter [2] so that it can be done within ~100 msec. Further development is under way for faster processing. Now SHIKA can be also used on BL41XU, a high flux beamline at SPring-8 with some adjustment for PILATUS3 (Detectris Ltd.) detector.

[1] N. K. Sauter, J. Hattne, R. W. Grosse-Kunstleve, and N. Echols (2013) Acta Cryst. D69 1274-1282, [2] G. Perrot, S. Domas, and R. Couturier (2013) Journal of Signal Processing Systems 1-6

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