# Software suite “SHITENNO” for automatically processing diffraction patterns in coherent X-ray diffraction imaging experiments at SACLA

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Using a diffraction apparatus named KOTOBUKI-1[1], we have been conducting cryogenic coherent X-ray diffraction imaging (cCXDI) experiments at X-ray free electron laser facility SACLA. In the experiments, we aim to visualize the internal structures of metal nano-particles and non-crystalline biological specimens such as cells and organelle at a resolution of a few tens nm. Sample particles scattered randomly on carbon or silicon nitride membrane are prepared under humidity controlled atmosphere and flash-cooled to the frozen-hydrated state [2]. The specimen membrane loaded into the vacuum chamber of KOTOBUKI-1 is raster-scanned against X-ray pulses at 1 Hz. Because of the wide range of diffraction intensity, we collect data using tandem detectors. One is an Octal multi-port CCD detector for high-angle diffraction patterns, and the other is a Dual multi-port CCD detector with attenuator for small-angle diffraction patterns. This experimental setup enables X-ray pulses to hit specimen particles at a rate of 30-100%. As a result, we obtain several terabyte of diffraction patterns during a few days. Now, we have been developing a software suite named SHITENNO for processing huge amount of diffraction patterns automatically and efficiently.

The SHITENNO suite treats diffraction patterns of HDF5 format, which are numbered according to X-ray shots in each measurement run. After subtracting dark current background of CCD detectors, we select diffraction patterns with significant level of intensity as expected from the scattering cross-section of particles by monitoring the sum of diffraction intensities in a specified small-angle area. Next, beam center positions in detectors for every diffraction pattern are determined. Based on the Friedel’s symmetry, we search beam center positions in detectors, which maximize the similarity in the diffraction patterns between a specified small-angle region and its centrosymmetry mate. Then, diffraction patterns from Octal and Dual detector are merged to a single file using geometrical parameters. The parameters are determined by approximating a diffraction pattern from a cube-shaped copper particle with an approximate dimension of 200 nm with sinc function. Merged diffraction data are submitted to the subsequent phase-retrieval calculation using the hybrid-input-output algorithm in combination with the shrink-wrap algorithm [3]. Immediately after a few hundreds of diffraction patterns per sample are recorded, the SHITENNO suite provides low resolution images of specimen particles within ten minutes.

In the presentation, we introduce the SHITENNO suite and demonstrate its performance in the cCXDI experiments at SACLA.

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[2] Y. Takayama & M. Nakasako, *Rev. Sci. Instrum.* **83**, 054301 (2012)
[3] T. Oroguchi & M. Nakasako, *Phys. Rev. E* **87**, 022712 (2013)