

Data collection and reduction program for sequential *in situ* powder diffraction experiments at non-ambient sample conditions at TPS 09A

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Abstract

In Taiwan Photon Source (TPS) 09A beamline, the high-resolution powder x-ray diffraction (HRPXRD) end-station was designed not only for static structure determination but also structure dynamics. Therefore, to integrate non ambient sample environment devices into beamline data collection program plays a crucial role. Three high/low temperature control devices (dynaflo cryostat, cryostream and hot air gas blower) and one battery charge/discharge device now are already opened for user operation, shown in Table 1. To enhance beamline performance and to simplify data collection and calibration process, a series of program were written, shown in Table 2. Based on two powerful programming languages, the Experiment Physics and Industrial Control System (EPICS) and Python, the automatically sequential *in situ* measurements are available. With these programs, the risk of human operation will be reduced and significantly improve the efficiency of data collection.

Table 1. The non-ambient condition of 09A end-station instruments.

Instrument	Dynaflow cryostat	Cryostream	Hot air gas blower	Autolab PGSTAT204
Non-ambient conditions	down to 4K	90K~500K	up to 900°C	potentiostat/galvanostat

Table 2. Data collection and reduction program

Data collection (Data reduction)	Detector and data type (2 θ range)	Special condition
mscan_py (mscan_py_anna)	MYTHEN 24K 1D pattern (1.8°~123.0°)	(1) TempControl : Cryostream, Dynaflo (2) AL_mscan : Autolab PGSTAT204
HT_mscan_py (HT_mscan_py_anna)	MYTHEN 24K 1D pattern (2.5°~78.0°)	TempControl : Blower
pdfscan (pdfscan_anna)	MYTHEN 24K 1D pattern (1.8°~147.9°)	For pair distribution function experiment
MCAscan (MCAcali, MCA_data)	Multi-Crystal Analyzer 1D pattern (2.0°~110°)	Ultra-high resolution experiment
PEscan (PEscan_AutoIntegrate)	Perkin Elmer XRD1611 2D pattern (~60°)	2D image measurement