Supplementary information

3. LVP Software

3.1. System control

All GSECARS instrument control is through the use of EPICS (Experimental Physics and Industrial Control System), which is a set of software tools and applications originally developed jointly by Argonne National Laboratory and Los Alamos National Laboratory for the purpose of controlling particle accelerators and large experiments. EPICS is a client/server system, where servers control the hardware and clients send commands to the servers and read values from the servers. Servers are also called Input Output Controllers, or IOCS. Clients include a number of operator interfaces for GUI based control. At GSECARS we use the Motif Editor & Display Manager (MEDM) graphical interface which allows staff to easily create, configure, and modify displays and then activate and connect displays to the actual hardware with no programming required. Clients connect to EPICS Process Variables (named objects) via the EPICS Channel Access network protocol. Clients only need to know the Process Variable name; no other knowledge of the hardware configuration is required. For scripting and programming, client applications can be written in virtually any language, including Python, IDL, C/C++, Matlab, the Linux and Windows shells, etc. This simple interface allows staff with little programming experience to easily write scripts to control complex experiments.

EPICS supports a wide variety of experimental hardware, and writing support for a new piece of equipment is typically not difficult. Each of the five GSECARS experimental stations has an EPICS IOC running on a VME crate with the real-time vxWorks operating system. These crates handle most of the motor control, analog and digital I/O, counter/timers, and many RS-232 devices. We also run IOCs on Windows and Linux machines. These IOCs control cameras and 2-D detectors using the EPICS areaDetector software (Rivers, 2018). They also control motors with Newport XPS motor controllers and a variety of other devices.

3.2. X-ray diffraction

3.2.1. EDXD

In EDXD applications, we use the Canberra solid state detector combined with the multichannel analyzer (MCA) to collect diffraction signals as a function of X-ray energy/wavelength. Amplified voltage pulses from the single element germanium solid state detector (SSD) are passed to a Canberra ADC and AIM Ethernet MCA in a NIM bin. The spectra from the AIM are read using an EPICS MCA record developed at GSECARS. The MCA record is controlled using a GUI written in IDL. Online analysis on energy and two theta calibration, cell parameter, volume, pressure can be easily performed using this program. Recently, we have installed Co_{57} and Cd_{109} radioactive sources into the SSD lead housing. The characteristic decay lines generated by the two sources are recorded in every single X-ray diffraction pattern, if needed, one can always re-check the energy calibration of the solid state detector to ensure reliable X-ray diffraction data. Both the energy calibration and the 2-theta calibration of the detector are performed by matching theoretical peak positions to each individual peak that were manually selected by the operator. The IDL detector control software can be configured to automatically erase the previously collected diffraction pattern on the display screen and start the next data collection after reaching the assigned data collection time. The patterns can also be saved automatically after each data collection, making it possible to collect a series of X-ray diffraction patterns and investigate the peak position, peak intensity evolution with other changing parameters during the experiment, e.g., time, pressure, and temperature.

3.2.2. ADXD

ADXD patterns are recorded at a desired fixed photon energy. Dioptas is a Python-based program for 2D area-detector X-ray diffraction data processing and exploration that was developed by C. Prescher at the GSECARS (Prescher & Prakapenka, 2015). One of the many advantages of this software, especially for the synchrotron beamline, is the capability of treating large amounts of data in an extremely fast and simple manner, compared to other software that we used in the past at the beamline, such as Fit2D. In addition to being a fast data reduction algorithm, the multifunctional graphical data exploration and instant display capability makes it a perfect tool for on-the-fly data processing during X-ray diffraction experiments and batch post-processing of large numbers of diffraction images. One important feature of Dioptas is the ability to calibrate almost any detector geometry, for example, beam center not included in the pattern, only a narrow "stripe" of partial rings recorded, or a large detector tilt angle. This capability is very useful when the imaging plate is positioned at a large angle relative to the incident X-ray beam as seen in our liquid structure measurements in a Paris Edinburgh cell.

3.3. Imaging

3.3.1. 2-D radiography

Imaging cameras for the LVP setup are controlled by the EPICS areaDetector software and displayed using the free and widely used software Image-J (Rasband, 1997). Image-J is a Java-based image processing program. The Java code "EPICS_AD_Viewer.java" is a plugin developed by Rivers et al. at the APS to display 2-D array image data. This plugin uses EPICS Channel Access to display images via waveform records that the NDStdArrays plugin sends to EPICS. Please visit http://cars.uchicago.edu/software/epics/areaDetectorViewers.html for more information regarding the Area Detector Viewers Plugin.

3.3.2. 3-D high-pressure tomography

An IDL routine "Tomo_collect_ad2" (Rivers, 2010) is used to control the HPXMT motor and the imaging camera for tomography data collection. The traditional stop-and-scan routine throughout the entire 180-degree data collection not only increases the total data collection time but also causes mechanical instability in the HPXMT apparatus especially when it is under high load. To eliminate the constant start-and-stop abrupt change in motor motion during high-pressure tomography, an on-the-fly data collection procedure has been implemented into the tomography data collection code Tomo_collect_ad2. With continuous motion of the rotation stage, the mechanical instability of the HPXMT apparatus has been greatly reduced.

For 3D high-pressure tomography image processing, reconstruction, and visualization, we utilize our own developed reconstruction software- Tomo_display (Rivers, 1998). It takes care of necessary data processing and corrections before reconstructing the images, including the dark current, the flat field, and the rotation center. The speed for reconstructing images has been greatly improved by using the new tomoRecon multi-threaded code (Rivers, 2012). It can reconstruct N slices in parallel on N cores in the workstation by using the high-speed Gridrec FFT algorithm. To reconstruct a dataset of 900 projections of an 1920 pixel x 1200 pixel image takes less than 60 s. Written in C++, the reconstruction code has an IDL user interface and can be run by users at their home institutions for free.

3.4. Deformation

Deformation experiments in the D-DIA apparatus require collection and calculation of multiple pieces of information about the sample during the deformation process, making it one of the most sophisticated experiments run at the synchrotron beamline. While monitoring the high temperature and the increasing hydraulic pressure of the advancing deformation pistons, one collects X-ray diffraction patterns to determine both the pressure and the stress level inside the sample. By driving in the scintillator and the imaging camera while opening the incident slits, X-ray radiograph images are then collected to measure the amount of strain that has built up inside the sample. In order to make the deformation experiments easier to control, we have created an IDL routine: "LOOP" to help the users switch the beamline hardware setups between X-ray diffraction and imaging mode and to collect X-ray diffraction images and X-ray radiographs of the sample automatically after switching setups. Once LOOP has been initiated, X-ray diffraction and imaging files will be collected and saved to the computer automatically.

3.5. Ultrasonic measurement, waveform generator, and oscilloscope control

Ultrasonic elastic wave travel time is determined by the pulse echo overlap method using the reflected signals from the buffer rod/sample and sample/backing plate interfaces. Individual Igor codes have been developed for travel time analysis. Both codes work on Windows and Mac machines.

The group led by Z. Jing of Case Western Reserve University has taken advantage of the new equipment and created a Python code to fit their experimental needs. Since travel time measurement of high-pressure melt is more difficult to perform due to the potentially unstable performance of the cell assembly, prompt measurement is a critical factor. One would want to minimize the time of keeping the cell assembly under high temperature. A program that switches the frequencies of the input signal then collects and saves the travel time data automatically has greatly improved the success rate of the experiments.

3.6. Acoustic emission data collection and analysis

InSite-Lab, developed by Itasca, is an integrated data acquisition, processing, management, and visualization software for acoustic emission applications. It has been applied to laboratory testing, rock physics, material testing, engineering, geotechnical, and concrete research. It has been commonly used in rock testing in the field or for localized rock mechanics experiments in the laboratories. We have been using InSite-Lab for our acoustic emission monitoring setup in the deformation DIA to record acoustic emission data during the experiments, and later analyze the waveforms to determine the location as well as the focal mechanism of a recorded event. The software can be configured to record the data stream continuously or to only record events that pass a certain energy threshold. The software can automatically record arrival times of the events, a crucial capability since thousands of events can often be detected within an experiment. Unfortunately, in some cases where the beginning of the waveform is unclear, the software tends to experience difficulties in determining the correct arrival-time. In this case, one will have to visually determine the arrival-time for each event. Application of the seismological algorithm hypoDD has shown great promise in greatly improving event location accuracy (Wang et al., 2017). InSite-Lab has a long list of analytical and displaying tools. Among the most frequently used are focal mechanism determination based on the first arrivals that have been measured, and power spectrum analysis for corner frequency analysis.

References

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