Initial testing of a Compact Crystal Positioning System for the TOPAZ Single-Crystal Diffractometer at the Spallation Neutron Source

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Abstract. A precise, versatile, and automated method of orienting a sub-millimeter crystal in a focused neutron beam is required for efficient operation of the TOPAZ Single Crystal Diffractometer at the Spallation Neutron Source at Oak Ridge National Laboratory. To fulfill this need, a Compact Crystal Positioning System (CCPS) has been developed in collaboration with Square One Systems Design in Jackson, Wyoming. The system incorporates a tripod design with six vacuum-compatible piezoelectric linear motors capable of $< 1 \mu m$ resolution. National Instruments LabVIEW provides a means of system automation while at the same time accommodating the modular nature of the SNS sample environment control software for straightforward system integration. Results from an ambient test at the Advanced Photon Source at Argonne National Laboratory will be presented.

1. Introduction
The TOPAZ single-crystal neutron diffractometer is scheduled to start commissioning early in 2010. It is designed to use crystal sizes that have been used traditionally by x-ray diffraction in order to maximize scientific impact. High solid-angle detector coverage on TOPAZ will allow the instrument to maximize the capture of neutrons scattered from a crystal sample, thus minimizing the number of crystal positions required to gather enough data to refine a crystal structure. As a result of this innovative detector orientation concept however, one will require a precise method of crystal orientation that will not interfere with detector coverage, operate in a vacuum, and still be versatile enough to cover as much of the crystal reciprocal space as possible.

A three-point, six-axis design was conceived and prototyped using high-resolution, piezoelectric actuators. The design was chosen due to its compact nature and the additional capability of translational motion. The design implements the six axes in the form of three vertical axes, and three horizontal axes, one of which is orthogonal to the other two. This motor concept, along with the unique three-point plate interface allows a flexibility that cannot be achieved with a traditional goniometer alone. In addition to this flexibility, the bulk of the positioner is offset from the sample position itself, minimizing the shadowing of positioner components in the detectors. A solid model of the design concept can be seen in Figure 1, and the prototype setup inverted on a table for characterization purposes can be seen in Figure 2. This prototype...
is capable of tilting up to a 15° incline in any direction, while still maintaining the sample in its original position. By adding a small rotational motor to this setup, this positioning concept compliments the TOPAZ instrument detector coverage. Complementary to the versatility of the hardware, control software was developed that can take full advantage of the positioner functionality. A GUI was designed using LabVIEW that is flexible, will integrate with the SNS control system, and provides a level of control abstraction that would be familiar to the crystallography community.

2. Control Method and Implementation

Basic motor control of the system is relatively trivial, however emulating the desired goniometric parameters is not. This challenge was solved by taking advantage of the tripod nature of the hardware and developing code that takes a vector along the sample pin as the normal of an abstract plane. This plane can then be used to determine the appropriate location of each of the tripod’s three points. This setup allows the use of traditional goniometer orientation angles, while at the same time preserving the flexibility of three axes of translational motion enabled by the hardware design. The aforementioned level of control abstraction is employed in the logical flow chart as seen in Figure 3.

Figure 1. A CAD generated solid model of the ambient design concept.

Figure 2. A photograph of the prototype. The prototype was inverted for testing purposes.

Figure 3. A flow chart describing the motor positioning algorithm.
A set of desired angles in a pre-programmed orientation space is determined by the user, then the software will determine a rotation matrix that represents the orientation space to be multiplied by the initial plane vectors. Once the new plane vectors are determined, the software then determines the new tripod positions to be set by the motors. Other features implemented into the software include the ability to save and recall orientation spaces, three axis translation for fine-tuning crystal location and the ability to have as many as ten unique rotation axes in one orientation space.

3. Ambient System Testing
Tests were performed at the Advanced Photon Source in Chicago, IL, USA to determine the functionality of the ambient system. The system was adapted to be installed at Sector 15 of the APS, in place of a traditional goniometer on an x-ray single-crystal diffractometer. The repeatability of the system was tested by mounting a test crystal on the positioner, centering the crystal sample in the x-ray beam, and then repeatedly tilting the crystal in between 0° and 5° around the beam axis.

As seen in Figure 5, Reflections were observed from the test sample. For every repetition back to zero, the same spot was located and a fit performed in order to determine the location of the reflection on the detector. The repeatability of the system is shown to be in the range of 30µm, although a general upward trend was observed. This trend was ultimately attributed to an insufficient holding force and low encoder resolution.

Figure 5. X-ray diffraction observed at 0°. Special thanks to X.P. Wang for test sample.

Figure 6. Reflection fit locations for repeated tilting from 0° to 5° and back to 0°.
4. Cryogenically Compatible CCPS
Testing has begun on a cryogenically compatible version of the initial design concept. The design tested at APS was adapted to use vacuum-compatible attocube Linear Nano-positioners with resistive encoders. These encoders allow better than 100 nm precision, depending on the setup of the encoder. In addition to the change in motors, a means of cooling the oriented sample needed to be addressed. Initially, a braid will be tested as seen Figure 8, but exchange gas methods could be implemented as well in the future.

![Figure 7. A CAD view of the Cryogenic CCPS. The different motors used provide the same functionality with a slight change in design.](image1)

![Figure 8. A photograph of CCPS during vacuum testing.](image2)

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