

**[s7.m0.p7] X-ray diffraction between 4K and 300 K on a four circle diffractometer equipped with a 2D detector.** R. Argoud<sup>b</sup>, P. Fertey<sup>a</sup>, P. Bordet<sup>b</sup> and J. Reymann<sup>a</sup>  
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Keywords: instrumentation, detectors.

A new low-temperature system for X-ray studies down to 4K has been developed. This new device has been specially designed to fit on a four circle diffractometer equipped with 2D detector.

The principle of this new device is inspired from the cryostat developed for a point detector four circle diffractometer [1]. The basic idea is to be able to move the crystal inside the cryostat, while the cryostat itself remains fixed. To achieve this goal, the crystal is mounted on a holder which is magnetically coupled to the diffractometer. This coupling is achieved by mounting a master magnet in place of the classical goniometer head. This magnet drives a slave magnet fixed on the crystal holder and therefore the crystal is indirectly oriented by the master magnet. Due to the 2D detection process, only two rotation axes are in principle needed to collect the whole accessible crystallographic data, simplifying the design of the sample holder. Therefore only the phi and omega rotations have been retained while the chi angle is fixed close to 45°. The data collection is carried out by performing omega-scans at different values of phi to improve the completeness.

The sample holder supporting the crystal is enclosed within a cryostat and the crystal is magnetically driven through the walls of the cryostat. To reach high temperature stability, a helium-bath cryostat has been chosen. The tails of the cryostat (room-temperature, liquid nitrogen and helium tails) have been specially designed to set the detector as close as possible from the sample to ensure the largest solid angle of detection.

Mechanical details on this new device (sample holder, cryostat, centering of the sample on the diffractometer...) as well as the performance of the apparatus (tested with yttrium iron garnet crystals) will be presented.

**[s7.m0.p8] A New "Open Source" Control-Program for Single Crystal Diffractometry.** Jürgen Kopf, *Institut für Anorganische und Angewandte Chemie der Universität Hamburg, Martin-Luther-King-Platz 6, D-20146 Hamburg, Germany.*

Keywords: control software in C++, Linux, open source.

Over the past decade we have been developing diffractometer control software that uses easy to learn pull-down menus, dialog-, alert- and file-selector-boxes. The program Y290 has been developed to control a still very reliable Hilger & Watts (Y290) four circle diffractometer via a new interface, using a 68008 microcomputer for serving the four stepper motors. The software, including the calls for the graphics system, was completely written in FORTRAN77 for an ATARI Mega ST<sup>2</sup>.

By isolating all modifications required to drive a different diffractometer, it was possible to re-write the same control program for a SYNTEX P21 diffractometer<sup>2</sup>. This program P21 used the so-called "SIEMENS-box" for driving the four DC motors.

Although an ATARI with 1 MB memory and only 8 MHz processor speed is completely sufficient for driving both diffractometers, a PC version under the operating system Linux was developed:

The new diffractometer control software is now completely written in C++ using the Qt class library, maintained and distributed by the Norwegian company Troll Tech<sup>3</sup>. Qt is a multi-platform C++ GUI toolkit that is supported on all major variants of Unix/X11 and Microsoft Windows. It is released in two different versions: the Qt Free Edition, which may be used free of charge for developing Free Software ("Open Source"), and the Qt Professional Edition. Since the new program Y290 uses the Qt Free Edition on Linux/X11, the source code will also be free software.

The power of this new program Y290 is derived from a sophisticated, menu-driven user interface which is much easier to use than the classical command-line input. The new version of Y290 is running over one year very reliable without any problems.

[1] Argoud R., Muller J., *J. Appl. Cryst.*, (1989), 22, 584-591.

[1] D. Abeln, J. Kopf, Abstract PS-02.06.01, IUCr XVI, Beijing, China, 1993.

[2] J. Kopf, D. Abeln, Abstract P21-10, ECM 16, Lund, Sweden, 1995.

[3] <http://www.troll.no/>