A CRYSTAL CENTRING SYSTEM WITH A FPGA BASED POSITION CONTROL APPROACH FOR EMBL BEAMLINES AT PETRA III

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Abstract

The EMBL is located at the DESY site in Hamburg and operates 5 beamlines at the DORIS III synchrotron. Additionally the EMBL Hamburg is in charge to build three beamlines at the new PETRA III high-brilliance synchrotron radiation source which will start user operation in 2009.

In this paper, an automatic crystal centring procedure i.e. the automatic positioning of a protein crystal on a diffractometer axis is presented. A reconfigurable FPGA based control solution is evaluated to monitor and analyze in real time beamline parameters for positional feedback. The system is integrated into the TINE control system and can be remotely controlled and configured.

The main elements of the control hardware are motion control electronics by *Beckhoff Automation GmbH*, piezo motor stages from *attocube systems AG* for fine adjustments and a *National Instrument* PXI crate equipped with a real time controller and R-series FPGA. The *Labview^{RT}* software to control the system is described as well as the adaptation of the hardware to various applications.

The solution is demonstrated on a test set-up and in the close future it will be transferred to an existing DORIS beamline used as test platform for PETRA III.

INTRODUCTION

PETRA III will be a new high-brilliance synchrotron radiation source on the DESY site in Hamburg. The core of the new EMBL facilities at PETRA III will be three undulator beamlines available to the international scientific community [1]. Two of these beamlines will be geared towards the use of very small and energy tunable X-ray beams for macromolecular crystallographic applications. On these beamlines the structure of micrometer-size protein crystals will be investigated for which the crystals have to be exposed to and rotated in a very intense and stable X-ray beam with a focus down to a few micrometers in size. For this, the crystals have to be mounted and centred on a rotation axis also with micrometer precision. They are inserted into tiny nylon loops (cryo-loops) or into micro-structured polyimide mounts which are fixed to pins that can be attached to the rotation axis by a magnetic cap. During mounting and the subsequent crystallographic measurement the crystals have to be cryogenically cooled by a cold nitrogen stream. The entire measuring procedure will be automated to a level that minimizes (and eliminates wherever possible) the need for user intervention. A new automated system will be described that provides the possibility to centre the crystal with the aim to use the beam position as feedback. For accurate crystal detection and centring the XREC crystal recognition software [2] is implemented into the system to recognize crystals and their shape inside the mount.

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THE SYSTEM

The control hardware is implemented first on a stand-alone test set-up that reproduces the beamline environment and then will migrate to the DORIS beamline BW7B for further tests until it will be implemented on the PETRA beamlines.

The mechanical test set-up consists of a spindle axis that rotates the crystal (φ axis) and an x-y translation stage that guarantees high precision crystal positioning into the plane orthogonal to the beam axis. These three axis are mounted on a horizontal translation (z axis) equipped with a Renishaw absolute encoder for higher accuracy (see Fig.1 for axis conventions).

Beckhoff control electronic is used to drive the motors of the φ and z axis and its core is an embedded PC running Windows CE real time system [3] that controls the electronic modules like I/O signals, motor drivers etc.

The core of the feedback hardware consists of a National Instrument PXI crate equipped with a real time controller and an R-series FPGA (Fast Programmable Gate Array). On this device a Labview control software is running that can obtain beamline parameters like beam intensity, beam position etc. and use these signals as feedback for the experiment. This device has been chosen for its low noise read-out of analog signals and its real time capability.

As optics for sample observation on the rotation axis, a GigE MPixel camera is used that gives the possibility of multicasting and a microscope is used with a motorized zoom with maximum magnification of 25 times. The field of view with no zoom is 4.25 x 4.25 mm^2 while at maximum zoom it is 0.3 x 0.3 mm^2 with a pixel size of 0.2 μm^2. These specifications can be adapted to the new PETRA III beamlines where the beam size can be down to 5 μm with accordingly small sample sizes.

In order to obtain a good image of the crystal the illumination has to be optimized. The system gives the possibility to use a combination of a coaxial 150 W cold light through the microscope and an in-house built backlight consisting of a strong LED and a lens to focus the light at the sample position. These lighting conditions give an intensive crystal illumination that makes the observation insensitive to external light sources specific to different beamline environments.

In order to reproduce the reduced visibility conditions in a cold nitrogen stream a cryo-cooling device is used that is controlled via TINE. In the following a list of the main hardware components with their specifications is presented while in Fig. 1 an image of the test set-up is shown.

- φ axis (rotation axis): Beckhoff DC motor (AM227M) with gearbox (Alpha, ratio 100) controlled via Beckhoff direct drive AX2000; sphere of confusion < 5 µm.
- X-Y movement: attocube piezo motors (ANT200-NUM) equipped with integrated absolute optical encoders with 10 nm resolution and controlled via attocube ANC350.
- Translation on the z axis: Phytron stepper motor with gear box controlled via a Beckhoff module (KL2541); Renishaw absolute optical encoder with 0.1 µm resolution.
- Prosilica camera GC138C, 1360x1024 pixel, GigE interface, 15 frames per second.
- Motorized (zoom and focus) microscope Optem 125C, 25:1 magnification, focusing lens (5 mm working distance), coaxial illumination (31 mm working distance).
- Motor control: Beckhoff embedded PC CX1020 running Windows CE.
- For signal processing and feedback software: NI PXI 8106 RT controller and NI FPGA 7831R.

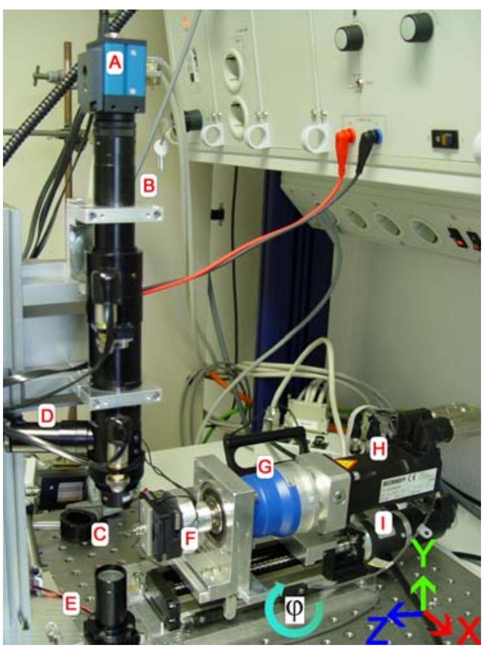

Figure 1: A) MPixel Camera, B) microscope, C) sample position and holder, D) coaxial light, E) backlight, F) x-y piezo motors, G) gearbox, H) rotation axis, I) motorized z translation. The axis convention is indicated in the right bottom corner; the X-ray beam axis will be along the x direction.

All the hardware has a server-client architecture implemented in the TINE control system [4]. Using the TINE multicast capability gives the possibility to run all clients simultaneously through the network.

Figure 2 shows a simplified scheme of the system architecture.

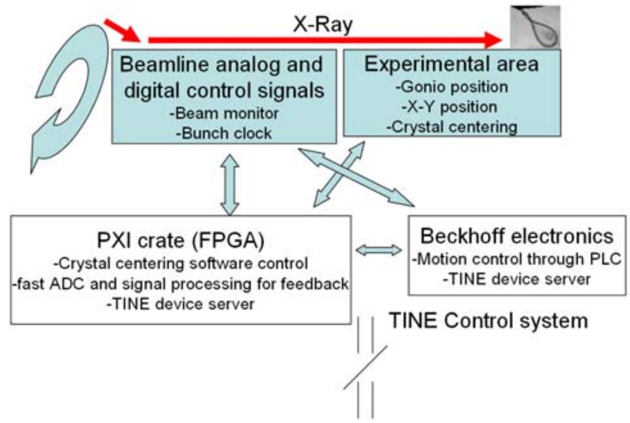

Figure 2: A simplified scheme for a possible architecture of the system at the beamline. The signals are processed by the PXI and the Beckhoff controller and exported as properties in TINE device servers. The feedback loops for the beamline control run on both controllers and they can interact between each other.

The centring control software will be integrated into a generic beamline control software. Its ultimate goal is to automate the entire experiment including the crystal mounting by a robotic sample changer [5]. The software will run in real time on the PXI crate controller where beamline parameters relevant for the experiment will be monitored and processed.

EXPERIMENTAL PROCEDURES

Crystal Centring

When a crystal is mounted on its support and installed on the rotation axis, the light is automatically adjusted using an algorithm based on finding the best contrast between the background and the crystal support. Pattern recognition algorithms detect the absence of the crystal or of the pin. The centring mechanism of the software provides a crystal mount centring using the NI Vision software algorithm tools to recognize the mount and centres it at a low level of zoom. This routine is based on a background subtracted image that separates the object to be studied from the background and thereby increases the repeatability of the algorithm. In a second step, the crystal mount centring is repeated at an intermediate level of zoom. In a final step, the crystal itself is detected and centred at the highest level of zoom inside its mount by using the XREC software. In Fig. 3 an example of a crystal detected by XREC is shown.

It is also possible to centre the crystal interactively without using the automatic crystal recognition software. For this, the user can adjust dynamically the zoom level, the lighting conditions and the crystal position within a prototype graphical user interface written in Labview (Fig. 4). This interface provides various options like digital zooming, line profile measurements, crystal area calculation and others. The image processing capability comprises also the possibility to automatically identify individual caps and their containers (baskets) through barcodes. In order to adjust the image during the dynamical zooming an auto focus option has been implemented based on a calculation of the standard pixel deviation performed on the fly during movements.

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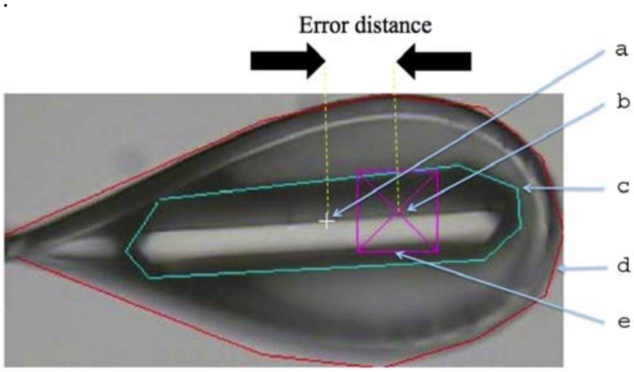

Figure 3: example of a crystal mounted in a cryo-loop automatically detected by XREC : a) real crystal centre, b) detected crystal centre, c) crystal polygons, d) loop polygons, e) detected crystal diameter. In this example, the difference between the crystal centre and the detected one is 10 µm.

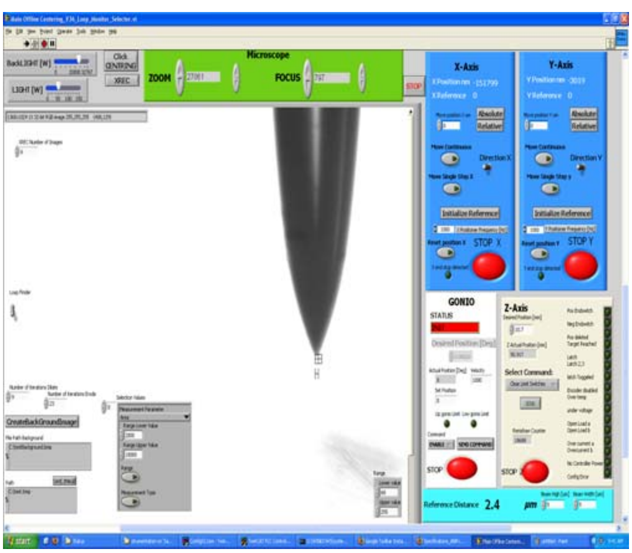

Figure 4: Labview prototype graphical user interface. The observed object is a needle used to calibrate the system (crosswire box is 5 µm).

FPGA Control

The FPGA acts as feedback control device and is especially useful when fast, noisy and highly sensitive electronic signals have to be recorded, digitized, possibly filtered and processed for closed loop operation. The device runs in real time at 40 MHz. The Labview code implemented on the FPGA can be exported in C to be potentially included in third party software.

In the present case, the feedback application for the FPGA will be the monitoring of a beam position signal and the immediate correction of possible changes acting on the x-y stage. An on-line correction of errors of the spindle axis during rotation can be also envisaged. This correction can be applied with a frequency adaptable to the experimental requirements and a maximum of 10 kHz.

As an alternative to the image processing on a control PC an option has been tested on the FPGA that offers different processing functionalities for video data coming from analog and digital cameras. The images can also be compressed, binned, filtered etc. The full resolution images are necessary for the algorithms to find the crystal position and used to locally display them at the beamline while compressed images are sent through the network in multicast mode.

SUMMARY AND OUTLOOK

The system is running successfully on a stand-alone set-up since a few months. Crystals can be automatically centred - the only input parameters are currently still the approximate crystal dimensions. Auto focus option and automatic crystal illumination adjustments are available. Feedback loops for adjusting the crystal position to an assumed X-ray beam position are implemented on the FPGA.

Future developments will include the optimization of the lighting conditions for different crystal sizes to improve the XREC centring reliability. An improved viewing system, on-axis with the X-ray beam, is planned that accounts in particular for the space restriction at the experimental endstation. After implementation of an X-ray beam position monitor on the beamline the FPGA based positional feedback can be further developed.

At the start of user operation on beamline BW7B, a highly automated experiment with a state-of-the-art automated crystal centring will be offered to the scientific user community.

REFERENCES

[1] Future service: EMBL@PETRA-III Project, http://www.emblhamburg.de/services/petra/index.html.

[2] http://www.embl-hamburg.de/XREC/.

[3] A. Pazos et al., "Embedded Distributed System Based on TINE and Windows CE", WEX04, proceedings of PCaPAC 2008, Slovenia.

[4] P. Duval, "TINE: An Integrated Control System for HERA", International Conference on Accelerator and Large Experimental Physics Control Systems, 1999, Trieste, Italy, p.526.

[5] U. Ristau et al., "Control of the new sample changer and Goniometer Hardware", WEP019, proceedings of PCaPAC 2008, Slovenia.