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Carbon nanotubes are nanometer sized channels that have a very high potential for applications such as selective chemical filtration or water desalination. For such purposes, large membranes of parallel nanotubes, where all metal-based catalyst particles potentially obstructing nanotubes have been removed, are needed.

An original experimental setup based on X-ray scattering and fluorescence has been designed to characterize membranes of arbitrarily large surface (cm² to m²) [1]. We are able to determine quantitatively the nanotube alignment in the membrane, the density of nanotubes and to check for the removal of metal-based nanoparticles. We will present the set-up, the models we developed to analyze experimental data and some results obtained on the set-up.

The set-up/modeling can also be adapted to others membranes than those of nanotubes, using small or wide angle scattering depending on the membrane composition.

It should be underlined than although the analysis requires complete orientational modeling within the framework of X-ray scattering theory, the set-up is designed for a non-specialist and could be used for instance on an industrial production line, automatic fitting of the data providing one with two-dimensional mappings of the density, chemical composition and nanotube orientation in direct space (figure).

[1] M. Huard, J. Cambedouzou, D. Petermann, P. Joly, G. Guillier and P. Launois *CNRS patent*, December **2010**.

**Keywords: X-ray, Diffraction, membrane**

## MS13.P04

**JBluIce-EPICS beamline control system for macromolecular crystallography**

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The report overviews the open-source JBluIce-EPICS control system [1] developed for the trio of highly successful GM/CA-CAT macromolecular crystallography beamlines in Sector 23 at the Advanced Photon Source. To make the control system fast, robust, intuitive for users and easily adaptable to new beamline developments, several technical solutions were implemented. First, the system consists of only two software layers, the EPICS backend providing robust control of distributed beamline hardware, and multiple graphical user interface (GUI) clients powered by Java Eclipse RCP. This provides the GUI with direct access to any advanced hardware features, such as on-the-fly scanning capabilities of motion controllers, and it is easy to add new features. Second, the GUI was chosen to conform to the task-oriented philosophy and to mimic the look and feel of the successful SSRL BluIce. Most users become proficient with the software within minutes. Third, JBluIce clients are designed to operate in parallel with other beamline controls, thus streamlining such staff tasks as beamline preparation and maintenance, operations auditing and user assistance. Further, JBluIce-EPICS deploys multiple plugins that can be written in any programming language, thus involving more staff in the development.

From the users' prospective, JBluIce provides: one-click change between 5, 10 and 20 μm beam sizes; one-click beamline energy change that may involve switching undulator harmonics, mirror lanes and beam realignment; automated diffraction rastering over multiple user-defined polygon shapes for finding small crystals and 'sweet' spots on poorly diffracting crystals [2], data collection along a vector [2]; automated on-the-fly fluorescent rastering with a shuttle scanning option, a faster and lower-irradiation compliment to the diffraction rastering [3]; fully automated fluorescence measurements for MAD that include signal optimization, fast on-the-fly energy scanning and automated adaption of scan range to chemical shifts [3]; fly-scan minibeam realignment; automated loop and crystal centering; controls for sample automounter; automated crystal screening; data collection auditing; remote access and more.

[1] S. Stepanov, O. Makarov, M. Hilgart, S.B. Pothineni, A. Urakhchin, S. Devarapalli, D.Yoder, M.Becker, C.Ogata, R. Sanishvili, N. Venugopalan, J.L.Smith, R.F.Fischetti *Acta Cryst.* **2011**, *D67*, 176-188. [2] M. Hilgart, R. Sanishvili, C. Ogata, M. Becker, N. Venugopalan, S. Stepanov, O.Makarov, J.L.Smith, R.F. Fischetti *J.Synch.Rad.* **2011**, *submitted.* [3] S. Stepanov, M.Hilgart, D.Yoder, O.Makarov, M.Becker, R.Sanishvili, C.Ogata, N.Venugopalan, D.Aragão, M.Caffrey *Acta Cryst.* **2011**, *D67, submitted.*

**Keywords: X-ray, biocrystallography, automation**

## MS13.P05

**Using GDA for novel data collection methods**

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Generic Data Acquisition (GDA, www.opengda.org) is the Java-based data acquisition software developed and used at the Diamond Light Source, the third generation synchrotron light source in the UK. GDA is designed to have a generic and flexible client-server architecture that has proven itself by running on almost all beamlines at Diamond and is now in use at several other synchrotrons.

Graphical user interfaces in the GDA client are controlled with intuitive motions to set up experiments. Standard oscillation experiments with crystals at a single position are now routine. In addition to the standard experiment, we have implemented automated techniques that are useful for evaluating crystals or larger sample holder (grid scan) or for collecting data sets along a three-dimensional crystal (line scan). Aided by the development of rapid detectors and suitable sample stages that allow continuous data collection during scans, these techniques have become even more powerful tools for examining samples in ways that would have been too tedious before their automation. The GDA client also aids in evaluation of the results, with feedback from external software presented graphically to the user. This immediate feedback and automation of the experiment are two ways that the beamline control software can contribute to improving the data collected at beamlines.

**Keywords: GDA, software, data_acquisition**

## MS13.P06

**CrysAlis[Pro]: facilitating variable temperature experiments**

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