feedback are at the cutting edge of technology, and the conceptual design of autonomous systems represents a research frontier in mechatronics. We expect that the current operator-assisting UMR will evolve into a system endowed with progressively increasing autonomy capable of significantly increasing reliability of protein micro-crystal harvesting and reproducibility of cryo-cooling. In addition, advanced micro-manipulation robotics will open the field to new science and emerging crystallization technologies of far reaching impact. Major improvements in operational precision have given the UMR the capability of manipulating crystals significantly smaller than 10 microns thus facilitating nano-crystallization, harvesting from micro-fluidics, nano-diffraction techniques and novel seeding strategies.

Keywords: robotic crystal harvesting, cryotechniques, automation

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Facilitating low volume protein crystallography set-ups using the mosquito® liquid handler

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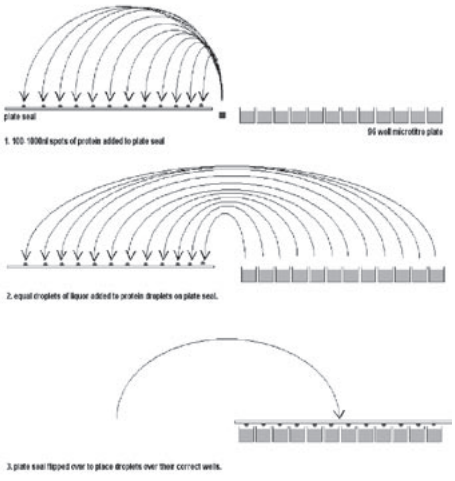
A prerequisite for efficient high throughput protein crystallisation screening is the accurate pipetting and positioning of the low volume drops used in hanging and sitting drop setups. Screening the many different conditions under which a protein crystal may form lends itself to automation, since it requires hundreds of similar experiments to be set up to find the few 'hits'. Automated solutions exist for low volume pipetting, however, the variable viscosities of protein and reservoir/screen solutions present significant challenges for many liquid handling systems. Another challenge is that of drop positioning. The mosquito® (TTP LabTech) offers fast positive displacement pipetting for accurate and reproducible aspiration and dispensing throughout the 50 nL - 1.2 μL range, producing CVs of < 8% at 50 nL irrespective of viscosity. This, plus its columnar arrangement of pipettes, allows it to automate hanging drop as well as sitting drop set-ups. Mosquito's micropipettes are also disposable, thus guaranteeing zero cross-contamination where required.



Keywords: protein crystallization, robots, laboratory automation

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A simplified unified approach for animations and movies using SBEVSL

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RasMol, Jmol, and PyMol, and many other molecular graphics programs are used to produce animations and movies. Each program takes a different approach making it necessary to use different commands and scripts when moving among programs, thereby making the development of lectures and tutorials more complex than necessary. The Structural Biology Extensible Visualization Scripting Language (SBEVSL) project is developing a common scripting language to access the common features of several molecular graphics packages. For some uses, the scripting language can be used as a black box, much the way we use Postscript for text documents, but, where feasible, SBEVSL is designed to be comprehensible to scientists by using simple menu-click-like commands and reasonable defaults. RasMol, PyMol and Jmol are being given "native" SBEVSL support and external translators will allow the approach to be applied to other packages, such as CCP4mg. For movies and animations the very useful but somewhat cryptic Jmol "moveto" command will be provided, but the SBEVSL version will be based on simple selection and recording of benchmark images using commands based on the PyMOL mset command combined with both time window and frame range based morphing. This work is part of the combined efforts of the SBEVSL groups at Dowling College and Rochester Institute of Technology. The people at Dowling are: Isaac Awuah Asiamah, Darina Boycheva, Georgi Darakev, Nikolay Darakev, John Jemilawon, Nan Jia, Petko Kamburov, Greg McQuillan, Daniel O'Brien, Georgi Todorov, Herbert J. Bernstein. The people at RIT are: Scott E. Mottarella, Brett Hanson, Charles Westin, Corey Wischmeyer, Paul A. Craig.
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Keywords: animation, graphics, script

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Remote data collection and rapid scheduling at the Molecular Biology Consortium beamline ALS 4.2.2

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The Molecular Biology Consortium consists of academic institutions throughout the USA and Taiwan. The cost of making regular synchrotron trips to the Advanced Light Source in Berkeley is not trivial and Beamline 4.2.2 initially addressed this issue with the addition of Service Crystallography. Since February of 2007 the MBC has also offered full remote collection capabilities and this has significantly improved access to the beamline. A Rigaku ACTOR sample mounting system is at the heart of remote operations and has been integrated into the Blu-Ice collection interface. Onsite computers installed with NX server software allow users to connect remotely via free client software. Sample mounting, exchanges,

unmounting and centering are all integrated into Blu-Ice through an intuitive custom robot tab; response over internet connections is reasonable from home (or café) wifi networks. Remote connection also allows data processing without the bottleneck of transferring the data home. Successful remote collection has enabled the MBC to institute an (almost) on-demand scheduling paradigm where members request beamtime as needed in blocks of time from 4 to 48 hours while beamline visits and Service Crystallography fill in the gaps. An MBC on-call list is available for beamtime to fill unused shifts and another ad-hoc beamtime request system is available for non-members. Remote collection has the benefit of easing access to the synchrotron beamline, encouraging the Mentor/Student relationship during data collection and provides a teaching platform that may otherwise be unavailable to crystallography labs.

Keywords: remote control, synchrotron radiation crystallography, X-ray data collection

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Femtosecond X-ray science at the Swiss Light Source

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Since mid-2006, 120 femtosecond synchrotron x-rays have been generated and used for a variety of experiments at the Swiss Light Source. Specifically, the source has been used to observe with high precision the structural dynamics of highly photoexcited semiconductor and semimetal crystals, allowing a more systematic study of the interaction mechanisms between electronic quasiparticles and phonon modes. We present here an overview of the techniques used to generate the femtosecond x-ray pulses, as well as an overview of the properties of these pulses relevant for experiments. We also demonstrate the successful use of the source to observe and control the femtosecond lattice dynamics of bismuth and tellurium.

Keywords: time-resolved x-ray diffraction, time-resolved effects, laser radiation

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WAXS as a novel tool in drug discovery

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A major advance in drug discovery has been the development of techniques to generate large libraries of target-focused probe chemicals. This development, in combination with the ever-increasing numbers of proteins entering screening programs via human genome expression profiling, has intensified the need for novel rapid screening techniques that can pinpoint those molecules with biologically relevant properties (such as knock-down or knockout activity). Most methods used to date rely on 1 of 2 strategies: either detection of physical binding or impairment of target function. The former class usually requires immobilization or tagging of 1 or more of the binding pairs and will identify ligands that may or may not impair protein activity, whereas the latter require specialized assays for each target function and may be less amenable to a high-throughput approach. Frequently, the functional binding of a small molecule to a protein is accompanied by a change in the structure of the protein. Wide-angle x-ray scattering (WAXS) is a sensitive probe of structural change in proteins and can detect protein changes across all relevant length scales. It addresses the shortcomings of existing screening techniques as it does not require either the protein or the ligand to be immobilized, labeled or modified in any manner and secondly it detects structural changes, not binding per se. We describe here the apparatus used at the Advanced Protein Source to collect WAXS data from small volumes of protein/protein-ligand solutions and proof-of-principle experiments that point towards the potential of WAXS as a novel routine screening tool for the detection of functional interactions between proteins and small molecule ligands for the purposes of drug discovery and development.

Keywords: wide-angle scattering, drug discovery, protein-ligand complexes

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Time-resolved photo-crystallographic investigation of metastable species

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X-ray crystallography is a ‘gold star’ analytical tool for obtaining structural information. Recently, crystallography has developed, so that structural information can be obtained as the reaction proceeds. One exciting development in this field is photocrystallography [1], which uses crystallography to monitor photochemical processes, in this case the formation of light-induced metastable species[2]. We now report the successful investigation of metastable species in a range of nickel complexes ([$Ni(NO_2)_2L$] L = (Aminoethyl)-pyroldine. In this investigation, the NO_2 ligand undergoes linkage isomerism [3] when irradiated by LEDs causing a change in coordination mode from the N-bound to the O-bound isomer. The new isomer is metastable and exists for a prolonged period of time. Using photocrystallography it is possible to monitor the new metastable conformation and percentage of converted NO2 ligands. The use of synchrotron radiation is key to this experiment as the high intensity allows for high quality results, short data collection times and the use of smaller crystals reducing the potential problem of only photoexcited surface ligands. The experimental techniques at Station 9.8 STFC and Station 11.3.1 ALS San Francisco will be discussed. The Pyrolidine complex produces a 40% conversion at 100K and is metastable for periods over an hour. In temperature experiments, the conversion percentage diminishes below 85K and above 120K. Higher conversions, with more extensive irradiating, were not explored due to crystal strain often resulting in the crystal fracturing.
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3. P. R. Raithby; Chem. Commun., 2006, page 2448-2450

Keywords: time resolved analysis, metastable structure