

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 photocystallography [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 $[\text{Ni}(\text{NO}_2)_2\text{L}]$ L = (Aminoethyl)-pyrrolidine. 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 photocystallography it is possible to monitor the new metastable conformation and percentage of converted NO_2 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 Pyrrolidine 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