Diffractions and Scattering Techniques

1936-Pos  Board B666
Secondary Structure Elucidation via X-Ray Cross Correlation Analysis
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We aim to measure substantial structural information via X-ray scattering in the absence of an ordered system. Instead of a crystal, which consists of N particles at a single orientation relative to the X-ray beam, our samples consist of N randomly oriented identical particles. Assume, in a given exposure, two (or more) photons scatter from the same particle in a time interval much less than the rotational diffusion time, i.e. while the particle orientation is fixed. These two photons are correlated via the structure of the particle. By time averaging intensity correlations from such measurements, one can hope to recover structural information of the single scatterer relative to the background of N randomly oriented scatterers. One can demonstrate the high-dimensional data obtained from such a correlation experiment exceeds that obtained with smallangle X-ray scattering measurements.
We have performed measurements on gold nanoparticle solutions at the Linac Coherent Light Source (LCLS) and are using them to identify and overcome the challenges involved in CXS experiments. Imperfections in detector geometry and electronic response can contribute to false correlations in the data; we are developing ways of identifying and removing these artifacts. We are simultaneously gaining the ability to recover protein secondary structural information from such data. Nanoparticle scattering will serve as a benchmark for an upcoming experiment at the Spring-8 Angstrom Compact free electron laser (SACLA), where we will attempt to measure correlated scattering from F-actin. Thereafter we hope to refine current models of the F-actin polymer by fitting them against our high dimensional data.

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Diffuse X-Ray Scattering for Ensemble Modeling of Crystalline Proteins
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Ensemble models of proteins have been developed using X-ray crystallography, and important advances have been made using translation-libration-screw motions of locally rigid domains, detection of alternative side chain conformations and contact networks, and X-ray restrained molecular dynamics (MD) simulations. Experimental validation is hindered, however, because Bragg peak data are unable to distinguish among different models that yield the same mean electron density. By contrast diffuse X-ray scattering reports on correlated motions and can be used to distinguish models that yield the same Bragg data. In particular, it has long been recognized that diffuse scattering could be used to validate MD simulations if adequate sampling of the conformational ensemble were achieved. We have performed a 1.1 microsecond MD simulation of crystalline Staphylococcal nuclease (SNase) and have evaluated the resulting ensemble us-

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SI-MoEXP: Software for Comparing Simulations to Experimental Scattering Data
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In recent years, high power neutron and X-ray scattering experiments have become important tools for investigating lipid bilayer systems found in biological membranes. These methods provide structural information for the bilayers by converting the scattering results into structure factors that provide some structural information, but are unfortunately limited in their scope and scale. The limitations arise due to the fluid nature of lipid bilayers, that unlike crystalline material do not have well defined periodic lattices and thus only produce broad peaked structure factors with essentially no long range order. A number of theoretical models have been developed to convert these structure factors into electron density and neutron scattering density functions across the bilayer, but these models are based on numerous assumptions and there is no way to confirm their correctness. To overcome the limitations of these models, the Simulation to Experiment (SI-MoEXP) software was developed. It converts simulation probability densities into structure factors for direct comparison with experiment, thus providing atomic level detail to the scattering results. Here we present an extended version of SI-MoEXP, rewritten in C++ and the ‘Qt’ GUI library in lieu of the original C/Tcl combination. A major extension has been added that reads molecular dynamics trajectories directly and calculates atomic probability densities across the bilayer. This eliminates much work for the user, and removes possible errors introduced through the calculation of the probability densities.

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Current Status of ABBIX Beamslines Developed for X-Ray Scattering and Macromolecular Crystallography at NSLS-II
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We present the current development status of the Advanced Beamslines for Biological Investigations with X-rays (ABBIX) at NSLS-II. This NIH-funded project includes an x-ray scattering beamline (LIX) and two macromolecular crystallography beamlines (FMX and AMX). User operations are scheduled to begin in 2016. Facilitating x-ray scattering studies on proteins in solution, lipid membranes and biological tissues, the High Brightness X-ray Scattering for Life Sciences beamline - LIX - will be equipped with a single long undulator (IVU23). Via a two-stage demagnification scheme it will produce beams down to a size of ~1 μm, and up to several hundred microns. With a broad energy range of 2.1 - 18 keV (0.7 - 5.9 Å) and capable of simultaneously collecting data on 3 detectors, it will support a variety of x-ray scattering measurements.
In the neighboring sector are the pair of MX beamlines, equipped with two identical canted undulators (IVU21). The beamlines' specializations are complementary. The Frontier Microfocusing Macromolecular Crystallography - FMX - will deliver a high photon flux of 10^13 ph/s at the Se K-edge into a spot of 1 μm width. It will cover a broad energy range from 5 - 30 keV, corre-

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Temperature-Pressure Phase Behavior of Triglycerides Revealed by Synchrotron X-Ray Scattering Studies
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Triglycerides, such as cocoa butter (also called theobroma oil), are widely used in food industry as they are a main part of foodstuff such as chocolate. This ingredient affects important properties like gloss, texture and mouth...