

MS38-O4**Time-resolved crystallography via an interlacing approach allows elucidation of milliseconds to seconds time delays**

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Time-resolved crystallography has recently seen a resurgence with the advent of very bright X-ray sources. However, time-resolved studies of enzymatic systems is often hindered by difficulties of acquiring time points which span the entire reaction coordinate pathway. Using a model system, fluoroacetate dehalogenase, to examine chemically triggered reactions, a proof-of-principle method using a chip as a fixed target, as well as a novel “*interlacing*” approach to data acquisition, timepoints ranging from milliseconds to several seconds can be acquired. Enabling >100k images to be collected within a few hours. Due to most enzymes not being susceptible to photoinduction, using caged fluoroacetate (2(4-hydroxyphenyl)-2-oxoethyl fluoroacetate), reaction initiation was achieved by photolytic cleavage via a femtosecond laser pulse of. Data collection was performed at both the P11 and P14 beamlines at the PETRA III synchrotron on sub-25-micron crystals. Multiple time points were collected spanning a range from milliseconds to several seconds producing well-resolved electron density maps ranging from 1.75-2 Å in resolution. Preliminary results showed significant structural changes in both the active site as well as dynamic changes in the cap domain, which support previously published results obtained by mutant trapping [1]. This newly developed method is highly flexible and can be used on numerous different enzymatic systems and can be adapted for use at XFELs as well as synchrotrons with bright microfocus beamlines.

References:

[1]. Kim, T.H. et al. (2017). The role of dimer asymmetry and protomer dynamics in enzyme catalysis. *Science*. 355(6322): eaag2355. Keywords: Time-resolved crystallography, crystallography, enzymology, method development

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MS38-O5**Ultrafast three dimensional X-ray imaging of strain dynamics in pulse-heated nanocrystals**

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The use of nanomaterials have become ubiquitous in several technological applications such as heat dissipation in semiconductors, thermal therapeutics via intensely heated nanofluids, and waste heat energy conversion via thermo-electric materials. Understanding the energy transport via lattice vibrations, under non-equilibrium conditions, play an integral role in the further maturing of these technologies. Three-dimensional imaging of the dynamical response of nanomaterials following ultrafast excitation can reveal energy transduction mechanisms, their dissipation pathways, as well as provide insight into material stability under conditions far from equilibrium.

Such dynamical behavior is extremely challenging to characterize especially at nano- to picosecond timescales. Recent advances in experimental techniques at x-ray synchrotron sources have enabled time-dependent measurements of three-dimensional strain evolution in nanomaterials. In particular, excitation by an ultrafast laser ‘pump’ and Bragg Coherent Diffraction Imaging (BCDI) using stroboscopic ‘probes’ of X-rays have been used to directly image lattice distortions within nanocrystals. Furthermore, with advances in high-performance computing and the use of machine learning approaches in material science, modeling and in-situ data analysis that complement BCDI measurements have provided crucial insights for energy research. Here, we provide a short review of recent progress in the integrated imaging (BCDI) and simulation (continuum and/or atomistic) approach that has been employed to characterize ultrafast lattice distortions on a wide class of material systems.

First, we discuss the laser pump excitation of zinc oxide nanocrystals to directly image the propagation of acoustic phonons at nanosecond timescales. By directly importing the experimentally reconstructed nanocrystal structure into a continuum deformation model, we identify the characteristic resonant modes excited by the laser pulse and characterize the electric potential gradients induced across the piezoelectric nanocrystal. Second, we characterize the deformation modes of core/shell semiconductor/metal nanorods following pulse-laser excitation of the metallic shell. An experimentally informed thermo-electromechanical continuum model elucidates the origin of the deformation modes observed experimentally. Third, we demonstrate inhomogeneous effects in lattice breathing at picosecond timescales, following femtosecond-pulse laser heating of bimetal core-shell nanocrystals, using multi-million-atom