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Recent advances and perspectives in fast time-resolved X-ray crystallography of proteins

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The purpose of this work is to outline the new developments and perspectives for time resolved X-ray scattering and diffraction analysis on a time scale from femtoseconds to milliseconds. The utilization of femtosecond laser pulses for the generation of X-rays has opened new opportunities for structural studies of fast kinetic processes. This new technology is essentially different from the operation principles employed at the synchrotron sources and the free electron lasers. The ELI beamlines facility is planned to start operation by the end of 2016 near Prague in Czech Republic. It will provide unique advantages for time-resolved crystallography based on laser-driven plasma X-Ray Source (PXS). The generated pulses will span approx. 100 fs with a repetition rate of 1 kHz. The scattered and diffracted X-rays by the sample will be counted using a Dectris Eiger 1M area detector, which operates at the same frame rate as the source, i.e. 1 kHz. The created setup can be combined with several pump probe lasers in order to study the fast kinetics of dynamic biological systems, for example the protein photo systems. Under the conditions of low flux, the generation of a crystallographic image requires several pulses to be obtained. Therefore, serial femtosecond crystallography at tabletop XPS sources is becoming feasible.

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Recent advances in crystallography for the future prospects

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New trends and perspectives in protein nanocrystallography are emerging at the intersection of advances in nanotechnology (Langmuir-Blodgett and Anodic Porous Allumina), functional (microarray, cell free expression and SNAP) and structural synchrotron radiation (third generation sources trillion times more brilliant and XFEL both requiring quite smaller crystals and Monte Carlo simulation) proteomics. It should be noted that nanocrystallography here does not refer to crystals of nanometer size or to nanodrop crystallization technology, but to the significant applications for crystallography emerging in our labs at the interface of Langmuir-Blodgett engineering, organic chemistry, molecular dynamics and label-free protein arrays, utilizing bacterial hell's gate globin, octopus rhodopsin, bovine cytochrome, human kinase, laccase and many other proteins. Molecular dynamics of proteins in aqueous environments are now routinely performed at an atomic level on the time scale up to several microseconds. MD simulations have been useful for predicting drug binding sites not available in protein X-ray structures, elucidating the origins of drug specificity, computing binding energies for ligand-protein systems and many other applications. Crystallographic methods have played an immense role in providing detailed biomolecular structural information and have been fundamental in the development of our understanding of the structure-function relationship. At the same time, crystallographic models can display an overreliance on static representations of biomolecular structure, despite the fact that biomolecules are intrinsically dynamic. MD simulations help to reveal these dynamics. The Monte Carlo approach has gained wide acceptance in multiple fields of natural science and technology as an effective tool for rapid integration in the highly dimensional spaces. It is extensively utilized in nuclear physics, molecular modeling, elementary particle physics, analysis of the diffraction data, etc. Here, we utilize the MC simulations in order to track the X-ray photons passage through protein crystals and their interactions. This work is an extension of the previous work, and it aims to improve our understanding of the exact organization of crystals, solute and salt orientation around the proteins. MD simulations of crystal lattices are carried out in different solutions as well as at different temperatures in order to understand the role of salts in crystal stability. In this research, we are planning to compare dynamics of lysozyme crystals obtained using the classical HD method, the LB method and the SG crystals. At the same time using Lomonosov supercomputer, we have developed a computational routine, which allows preparing molecular geometries corresponding to arbitrary protein crystals optimized and sampled using MD simulations and subsequently simulate initial processes of radiational damage in them by means of our Monte Carlo approach.

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