MS38-O2

Serial Crystallography - Exciting possibilities for time resolved Structural Biology

Dominik Oberthuer[1]

1. Center for Free-Electron Laser Science - Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany

email: dominik.oberthuer@desy.de

An overview will be given on recent developments in XFEL- and synchrotron based serial crystallography towards time-resolved structural biology. Methods will be presented and discussed, as well as limitations and future prospects.

Keywords: Serial Crystallography, Time Resolved Crystallography, Structural Biology

MS38-O3

Short and long-term structural effects of terahertz radiation on cryo-cooled bovine trypsin crystals

Viktor Ahlberg Gagnér[1], Ida Lundholm[1], Maria-José Garcia Bonete[1], Helena Rodilla[2], Vitali Zhaunerchyk[3], Gleb Bourenkov[4], Thomas Schneider[4], Jan Starke[5], Gergely Katona[1]

1. The Department of Chememistry and Molecular Biology, The University of Gothenburg, Gothenburg, Sweden
2. Terahertz and Millimetre Wave Laboratory, Chalmers University of Technology, Gothenburg, Sweden
3. Department of Physics, The University of Gothenburg, Gothenburg, Sweden
4. EMBL Hamburg c/o DESY, Hamburg, Germany
5. Terahertz and Millimetre Wave Laboratory, Chalmers University of Technology, Gothenburg, Sweden

email: viktor.ahlberg.gagner@gu.se

The use of non-ionizing Terahertz (THz) radiation in technology is a new growing field. New methods utilise THz radiation in for instance security screening at airports and border controls, and in medical diagnostics [1]. In contrast to x-rays, the THz radiation can non-destructively screen medical patients. In addition, the radiation generates a high contrast in soft tissue due to water absorption, and has higher spatial resolution compared to MRI and ultrasound [2]. Albeit non-ionizing, research have shown that THz radiation might still induce changes biomolecules due to collective oscillations [3]. In addition, a report from the U.S. National Toxicology Program states that non-ionizing radio waves from cell phones might have a cancerous effect. Therefore, it is imperative to study this protein-radiation interaction, not only for the sake of potential adverse effects biological systems, but also for the new insight this information provide to protein - light interactions.

To research the effect of THz interactions, bovine trypsin was crystallized, flash-cooled to 100 K, and studied in a pump-probe x-ray crystallography experiment. During the experiment, the crystals were pumped with 0.5 THz radiation, for 22.5 ms, and simultaneously probed with 14 KeV x-rays during 25 ms, with no THz radiation at half of the duty cycle. The data (diffraction up to 1.15 Å) show differences in the isotropic and anisotropic contribution of the atomic displacement parameter (ADP) tensor, for individual atoms. The differences are detected during both short term timescales (differences between odd and even frames), and long term timescales (differences between THz-radiated and reference crystals). Additionally, the ADP tensor forms functional links to seemingly unrelated parts of the protein. In general, these data indicate a structural order which is induced by the THz radiation, in contrast to the general disorder, expected from an increased thermal energy.

References:

[1] Wilmink G.J. & Grundt J.E. (2011). J. Infrared Milli. Terahz. Waves. 32, 1074–1122

[2] Hao, Y. & Yang, S. (2016). Design of CMOS Millimeter-Wave and Terahertz Integrated Circuits with Metamaterials, pp. 6. Boca Raton: CRC Press

[3] Lundholm, I.V. et al. (2015). Structural Dynamics. 2, 054702

Keywords: Crystallography, THz radiation