

Tracing of transient species via combined crystallographic and spectroscopic techniques – new perspectives from the XFEL Centers of Excellence initiative

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Whereas studies of light-induced effects in solutions are rather well-developed nowadays, the solid-state investigations of this kind are much more demanding, thus less established. Nevertheless, solid-state materials applications are of great and constantly increasing significance, ranging from sensors, optoelectronic devices and ultra-high capacity data storage media, to environmental and biomedical applications. Therefore, a considerable volume of effort should be dedicated to studies of materials in their technologically-applicable solid-state form. In this respect, single crystals are unique due to well-defined three-dimensional structure. This property makes them excellent model systems to mimic real-world situations, but also to supplement the solution-sample studies, or model the inter-surface environment. Since light-induced processes cause structural distortions (new bond formations, atom oxidation state changes, etc.), in the case of crystals they can be explored via X-ray diffraction techniques.

In this contribution the current possibilities of (time-resolved) photocrystallography for small-molecule crystals will be presented. Investigations of photoswitchable nitro complexes of transition metals will serve as examples of static photocrystallographic research [1,2]. In turn, the results of time-resolved synchrotron studies dedicated to photoactive transition-metal complexes in the solid state will show the use of the time-resolved Laue technique to track photo-induced short-lived excited states in molecular crystals [3,4,5]. Structural changes observed 100 ps after the excitation will be presented. Additionally research perspectives emerging once XFEL radiation is applied will be discussed. In this context the network of X-ray Free-Electron Laser Centers of Excellence (XFEL CoE), which has been established this year to provide substantive and organizational support to the Polish scientific community in the use of the European XFEL (EuXFEL), will be presented.

Acknowledgements: SONATA BIS (2020/38/E/ST4/00400), NSC (Poland), Support for Polish EuXFEL users–Supervision, Part II (2022-26), Ministry of Science and Education (Poland), South African National Research Foundation (137759), Advanced Photon Source, BioCARS beamline (R24GM111072) NIH (U.S.). Development of TR setup at BioCARS possible via collaboration with Philip Anfinrud (NIH/NIDDK).

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