

Low background pink beam serial crystallography

A. Meents^{1,2*}, M.O. Wiedorn¹, V. Srajer³, R. Henning³, I. Sarrou¹, J. Bergtholdt¹, M. Barthelmess¹, P. Reinke⁴, D. Dierksmeyer¹, A. Tolstikova¹, S. Schaible², M. Messerschmidt⁵, C.M. Ogata⁶, D.J. Kissick⁶, M. Taft⁴, D. Manstein⁴, J. Lieske², D. Oberthuer¹, R.F. Fischetti⁶, H.N. Chapman¹.

¹Center for Free Electron Laser Science (CFEL), Luruper Chaussee 149, 22607 Hamburg, Germany.

²Deutsches Elektronen Synchrotron (DESY), Photon Science, Notkestrasse 85, 22607 Hamburg, Germany.

³The University of Chicago, Center for Advanced Radiation Sources, 9700 South Cass Ave, Argonne, 60439 Illinois, USA.

⁴Medizinische Hochschule Hannover (MHH), Institut für Biophysikalische Chemie, Carl-Neuberg-Str. 1, 30625 Hannover, Germany.

⁵National Science Foundation BioXFEL Science and Technology Center, 700 Ellicott Street, Buffalo, New York 14203, USA.

⁶Advanced Photon Source, Argonne National Laboratory, 9700 S. Cass Ave Lemont, 60439 Illinois, USA.

Serial X-ray crystallography allows macromolecular structure determination at both X-ray Free Electron Lasers (XFELs) and, more recently, synchrotron sources. Whereas the short pulse duration at XFELs allows for experiments with femtosecond time resolution, the time resolution for serial synchrotron crystallography experiments has been limited to millisecond time scales with monochromatic beams. Using the polychromatic, “pink”, beam increases the photon flux by more than two orders of magnitude.

Using a setup optimized for very low scattering background we collected polychromatic datasets from four different protein samples at the BioCARS instrument at the APS. Complete datasets were obtained by merging pink beam diffraction patterns from many crystals, each collected with a single 100 ps X-ray pulse exposure per crystal. In contrast to serial crystallography experiments with monochromatic radiation, data from only 50 crystals were required to obtain complete datasets. The high quality of the diffraction data highlights the high potential of this method for studying irreversible enzyme reactions at sub-microsecond timescales using high-brightness X-ray facilities.