Ultrafast coherent diffraction imaging with a soft X-ray free-electron laser

Henry N. Chapman[1,5*], Anton Barty[1], Michael Bogan[1], Sébastien Boutet[1,6,7], Matthias Frank[1], Stefan P. Hau-Riege[1], Stefano Marchesini[1,5], Bruce Woods[1], Saša Bajt[1], Richard A. London[1,5], Elke Plönjes-Palm[2], Marion Kuhlmann[2], Rolf Treusch[2], Stefan Düsterer[2], Thomas Tschentscher[2], Jochen Schneider[2], Eberhard Spiller[3], Thomas Möller[4], Christoph Bostedt[4], Matthias Hoener[4], David Shapiro[5], Keith Hodgson[6], David van der Spoel[7], Florian Burmeister[7], Magnus Bergh[7], Carl Caleman[7], Gösta Huldt[7], Marvin Seibert[7], Filipe Maia[7], Richard W. Lee[1,7], Abraham Szöke[1,7], Nicusor Timneanu[7], and Janos Hajdu[6,7*].

[1] University of California, Lawrence Livermore National Laboratory, 7000 East Avenue, Livermore CA 94550, USA.
[2] Deutsches Elektronen-Synchrotron, DESY, Notkestraße 85, D-22607 Hamburg, Germany
[3] Spiller X-ray Optics, Livermore CA 94550, USA.
[4] Institut für Atomare Physik, Technische Universität Berlin, Hardenbergstraße 36, PN 3-1, 10623 Berlin, Germany
[5] Center for Biophotonics Science and Technology, University of California, Davis, 2700 Stockton Blvd., Suite 1400, Sacramento, CA 95817, USA.
[6] Stanford Synchrotron Radiation Laboratory, Stanford Linear Accelerator Center, 2575 Sand Hill Road, Menlo Park, California 94305, USA.
[7] Laboratory of Molecular Biophysics, Institute of Cell and Molecular Biology, Uppsala University, Husargatan 3, Box 596, S-75124 Uppsala, Sweden

Diffraction microscopy is an imaging mode that relies on the numerical inversion of a diffraction volume to recover the object function, and offers the potential for high-resolution aberration-free diffraction-limited 3D imaging. Theoretical studies and simulations predict that with a very short and very intense coherent X-ray pulse a single diffraction pattern may be recorded from a large macromolecule, a virus, or a cell without the need for crystalline periodicity. Measurement of over-sampled X-ray diffraction patterns permit phase retrieval and hence structure determination. Although individual samples will be destroyed by the X-ray pulse, a three-dimensional data set could be assembled when copies of a reproducible sample are exposed to the beam one by one.

Here we report the first experimental verification of the principle of flash diffraction imaging using a soft X-ray free-electron laser. The results show that an interpretable diffraction pattern can be obtained before the sample turns into a plasma when exposed to an intense 25 fs long photon pulse at 32 nm wavelength (focused to a peak intensity of up to 10^14 W/cm2). Significantly, the image we obtain by phase retrieval and inversion of the diffraction pattern shows no discernible sign of damage, and the object can be reconstructed to the resolution limit. Damage occurs only after the pulse traverses the sample. A second exposure shows scattering from the hole that was created by the first pulse.

These results provide experimental evidence for the basic principle of flash imaging, and have implication for studying non-periodic molecular structures in biology, and in any other area of science and technology where structural information with very high spatial and temporal resolution is valuable.

* E-mail: barty2@llnl.gov