First published results from new X-ray laser

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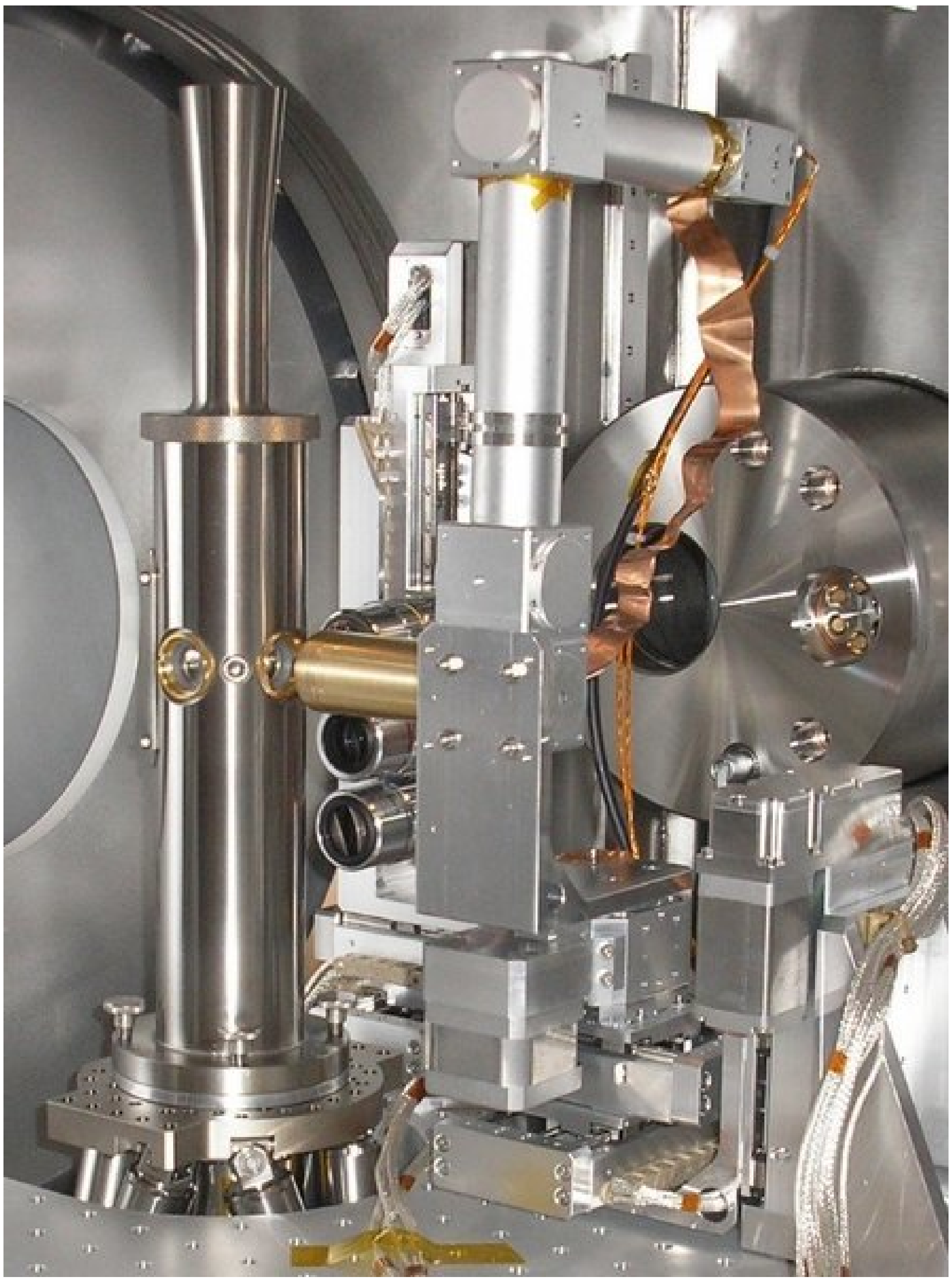

View into the experimental chamber of the SPB/SFX instrument in which the experiments were performed. Important contributions to the injection instrumentation were made by scientists from the Max Planck Institute for Medical Research, whose pioneering work on injection of samples into X-ray beams was crucial to these XFEL measurements, as well as to many previous measurements at first generation XFELs. The Max Planck Society is part of the user consortium that provides instrumentation and personnel for the SPB/SFX instrument at the EuXFEL where these experiments were performed. Credit: Max Planck Society

With the publication of the first experimental measurements performed at the facility, the European X-ray Free-Electron Laser (EuXFEL) has passed another critical milestone since its launch in September 2017. It is the first of a "next generation" of XFELs that offer much more rapid data collection than was possible before. As the EuXFEL delivers X-ray pulses at the almost unbelievable rate of one million pulses per second, experimental measurements can be completed more quickly, allowing more experiments to be carried out per year. It was not obvious however, that current measurement techniques would be able to handle this deluge of X-ray pulses. Researchers at the Max Planck Institute for Medical Research in Heidelberg and from Rutgers University in Newark, USA, working with an international team of collaborators and scientists from DESY and the EuXFEL, have now demonstrated that not only can this be done, but also that high quality structural information on biological molecules is obtained. This is a breakthrough for the facility and for structural biologists using XFELs worldwide.

X-ray free-electron lasers (XFELs) allow researchers to obtain three-dimensional images of biological molecules by means of snapshot X-ray exposures lasting mere femtoseconds. Such images can be combined to deliver "movies" of molecules on the incredibly brief time scale of chemical reactions. This provides new insights into the nanoworld that are not only important for basic sciences ranging from biology to physics, but also help advance developments towards new and better drugs, batteries and storage media, and many other things.

Unfortunately, only a handful of XFELs exist worldwide, and only a fraction of the experiments that scientists want to do can be accommodated. This is also because the original, "first generation" XFELs deliver X-ray pulses at only about the frame rate of a TV camera, around 50 times per second. However, by using superconducting resonator to accelerate the electrons that are used to produce the X-rays, new generation XFELs such as the European XFEL (EuXFEL) deliver as many as one million pulses per second. The excitement in the community was therefore huge when the EuXFEL was inaugurated less than a year ago.

The new possibilities of data collection at high repetition rate XFELs are, however, accompanied by entirely new challenges for the scientists doing the experiments. The same extraordinarily intense femtosecond XFEL pulses that allow tiny objects to be studied necessarily also heat and eventually vaporize the sample. This is not a problem in and of itself, since the femtosecond X-ray snapshot has been completed long before sample blows apart. Extreme care must be taken, however, that the damage from one XFEL pulse does not disturb the sample to be probed by the next pulse. The sample medium must therefore be moved between X-ray pulses, so that the XFEL beam never hits close to the same place twice. At 50 pulses per second this is easily done; but with only a millionth of a second between pulses it was not obvious that it would ever be possible.

Successful experiments

In June 2018, scientists from the department of Biomolecular Mechanisms at the Max Planck Institute for Medical Research in Heidelberg together with an international research team, led by Ilme

Schlichting, director at the Max Planck Institute, performed one of the first experiments at the EuXFEL. The team confronted and mastered the challenges associated with the rapid arrival of the EuXFEL pulses, successfully obtaining and fully analyzing high quality data for a variety of protein molecules.

"In our paper, we show that, under the current conditions, the shockwave induced by one XFEL pulse does not influence the sample probed by the next pulse, even when that second pulse arrives only one millionth of a second later," says Thomas Barends, a research group leader at the MPI and one of the corresponding authors. The data are of sufficiently high quality to also allow detailed analysis of a previously uncharacterized sample. This is a milestone for the facility and of great practical significance, given the rapidly growing demand for XFEL beam time. "The EuXFEL allows us to collect more data in much less time, enabling us to do novel science" says Marie Grünbein, first author of the publication and a Ph.D. student at the Max Planck Institute in Heidelberg.

More information: Marie Luise Grünbein et al. Megahertz data collection from protein microcrystals at an X-ray free-electron laser, *Nature Communications* (2018). DOI: 10.1038/s41467-018-05953-4

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