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Femtosecond Nanocrystallography with X-ray Free-Electron Lasers[1]

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The ultrafast pulses from X-ray free-electron lasers have opened up a new form of protein nanocrystallography. The X-ray pulses are of high enough intensity and of sufficiently short duration that individual single-shot diffraction patterns can be obtained from a sample before significant damage occurs. This "diffraction before destruction" method may enable the determination of structures of proteins that cannot be grown into large enough crystals or are too radiation sensitive for high- resolution crystallography. Ultrafast pump-probe studies of photoinduced dynamics can also be studied. We have carried out experiments in coherent diffraction from protein nanocrystals, including Photosystem I membrane protein, at the Linac Coherent Light Source (LCLS) at SLAC. The crystals are filtered to sizes less than 2 micron, and are delivered to the pulsed X-ray beam in a continuously flowing liquid jet. Millions of diffraction patterns were recorded at the LCLS repetition rate of 60 Hz. Tens of thousands of the single-shot diffraction patterns have been indexed, and combined into a single crystal diffraction pattern, which can be phased for structure determination and analysed for the effects of pulse duration and fluence. Experimental data collection was carried out as part of a large collaboration involving CFEL DESY, Arizona State University, Max Planck Institute for Medical Research, University of Uppsala, SLAC, LBNL, LLNL, using the CAMP apparatus which was designed and built by the Max Planck Advanced Study Group at CFEL.

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