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Data collection strategies for time-resolved X-ray free electron laser diffraction, and 2-color methods.[1] CHUFENG LI, KEVIN SCHMIDT, JOHN SPENCE, Arizona State University, DEPARTMENT OF PHYSICS, ARIZONA STATE UNIVERSITY TEAM — We compare three schemes for time-resolved X-ray diffraction from protein nanocrystals using an X-ray free-electron laser. We find expressions for errors in structure factor measurement using Monte Carlo pump-probe method of data analysis with a liquid jet, the fixed sample pump-probe (goniometer) method, and a proposed two-color method. Here, an optical pump pulse arrives between X-ray pulses of slightly different energies which hit the same nanocrystal, using a weak first X-ray pulse which does not damage the sample. (Radiation damage is outrun in the other cases.) This two-color method, in which separated Bragg spots are impressed on the same detector readout, eliminates stochastic fluctuations in crystal size, shape, and orientation and is found to require two orders of magnitude fewer diffraction patterns than the currently used Monte Carlo liquid jet method, for 1% accuracy. Detailed simulations provided for cathepsin B and IC3 crystals. While the error is independent of the number of shots for the dose-limited goniometer method, it falls off inversely as the square root of the number of shots for the two-color and Monte Carlo methods, with a much smaller pre-factor for the two-color mode, when the first shot is below the damage threshold.

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