ID: 1892 - WEPSO63 Extension of Sase Bandwidth Up to 2 % as a Way to Increase Number of Indexed Images for Protein Structure Determination by Femtosecond X-ray Nanocrystallography at the European XFEL

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Abstract Experiments at the LCLS confirmed the feasibility of femtosecond nanocrystallography for protein structure determination at near-atomic resolution. These experiments rely on X-ray SASE pulses with a few microradians angular spread, and about 0.2 % bandwidth. By indexing individual patterns and then summing all counts in all partial reflections for each index it is possible to extract the square modulus of the structure factor. The number of indexed images and the SASE bandwidth are linked, as an increasing number of Bragg spots per individual image requires an increasing spectral bandwidth. This calls for a few percent SASE bandwidth. Based on start-to-end simulations of the European XFEL baseline, we demonstrate that it is possible to achieve up to a 10-fold increase of the electron energy chirp by strongly compressing a 0.25 nC electron bunch. This allows for data collection with a 2 % SASE bandwidth, a few mJ radiation pulse energy and a few fs-pulse duration, which would increase the efficiency of protein determination at the European XFEL. We prove this concept with simulations of photosystem-I nanocrystals, with a size of about 300 nm.

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Main Classification Applications of FELs