



Contribution ID: 99

Type: Contributed poster

Revealing the nanoscale structure of viruses with XFEL pulses

Monday 25 June 2018 18:45 (15 minutes)

Imaging individual biological particles, such as macromolecules or viruses, at high resolution is one of the most attractive challenges for x-ray free electron lasers (XFELs). It was predicted that diffraction patterns from single particles can be measured in “diffraction before destruction” experiments at XFELs before the sample is destroyed by intense radiation, and hence their damage-free structure identified. Substantial technical achievements have now made it possible to perform such measurements. However, the limited resolution of the reconstructed biological samples demonstrated so far demands further theoretical and experimental efforts to establish single particle imaging (SPI) techniques at XFELs [1]. Therefore, alternative methods for structural characterization of nanoscale objects at XFELs are of great interest.

Here we apply the fluctuation x-ray scattering (FXS) technique, which is based on the detection and analysis of angular correlations of scattered photons [2]. We use extremely bright and ultrashort pulses from an XFEL to measure correlations in x-rays scattered from individual biological particles. This allows us to go beyond the traditional crystallography and SPI approaches for structure investigations. We employ FXS to recover the three-dimensional (3D) structure of aerosolized virus particles from x-ray diffraction data measured with the Linac Coherent Light Source (LCLS) [3, 4]. We determine angular correlation maps, which comprise a complex fingerprint of the whole 3D structure of a virus. Our results of model-based structure analysis and *ab initio* structure recovery reveal deviations of the virus structures from the expected icosahedral shape [4]. Our findings demonstrate substantial potential of FXS for the future studies of structure and dynamics of biological samples and nanoparticles with an XFEL.

[1] A. Aquila et al., *Structural Dynamics* **2**, 041701 (2015)

[2] R. P. Kurta, M. Altarelli and I. A. Vartanyants, *Advances in Chemical Physics* **161**, pp.1-39 (2016)

[3] J. J. Donatelli, P. H. Zwart and J. A. Sethian, *Proc. Nat. Acad. Sci.* **112**, 10286 (2015)

[4] R. P. Kurta et al., *Phys. Rev. Lett.* **119**, 158102 (2017)

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Session Classification: Poster session