



Contribution ID: 21

Type: **Poster**

Following the diffusive processes during a non-classical protein crystallization via neutron spectroscopy

Wednesday, 9 June 2021 14:40 (20 minutes)

Following molecular dynamics during the temporary evolution of kinetically changing samples is a major challenge. With recent developments of analysis frameworks, accessing the short-time self-diffusive properties of protein solutions by measuring specific energy transfers via neutron backscattering, kinetically changing samples can be investigated. The immobile fraction, determined by multi-dimensional fits of full QENS spectra, can be assigned to proteins in a gel-like state or in crystals [1]. Using time-dependent neutron spin echo measurements at different momentum transfers q , we access the collective diffusion during the crystallization process in different phases of the sample.

Here, we discuss the results of a recent protein crystallization study. CdCl_2 induces a non-classical crystallization process [2,3] of BLG with a metastable intermediate phase. We investigated the short-time collective and self-diffusion of BLG by neutron spin-echo (IN11), FWS and QENS (IN16b), respectively, of the crystallization process for different sample conditions. Combining the different results, a consistent picture of the process can be obtained, which differs significantly from classical BLG crystallization induced by ZnCl_2 [1]. This implies a strong influence of seemingly subtle cation-specific effects on protein crystallization.

[1]C. Beck et al., Cryst. Growth Des. 2019

[2]A. Sauter et al., J. Am. Chem. Soc. 2015

[3]A. Sauter et.al., Faraday Discuss. 2015

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Session Classification: Poster Session

Track Classification: Protein structure, function and dynamics