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

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Following dynamics *during* 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 (FWS) via neutron backscattering, kinetically changing samples can be investigated. More detailed information (internal dynamics and immobile fraction of the proteins) can be extracted from full QENS spectra obtained with a floating average with a lower kinetic time resolution. The immobile fraction, determined by multi-dimensional fits, can be assigned to proteins in a gel-like state or in crystals [1]. Here, we discuss the results of a study performed *during* crystallization. CdCl_2 induces a non-classical crystallization process [2,3] of β -lactoglobulin (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 drawn, 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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