ESRF	**Experiment title:** Structural dynamics investigations of intrinsically disordered proteins: hydrogel dynamics	**Experiment number**: LS-2808
Beamline: ID09	**Date of experiment**: from: 07.06.2018 to: 12.06.2018	**Date of report**: 28.02.2020
Shifts: 9	**Local contact(s)**: Mathias Sander	*Received at ESRF:*

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Report:

Actual Experiment

The structural dynamics of protein hydrogel samples were investigated in the TR-WAXS setup (Fig 1(a)). The measurements were performed using the pink beam optics at 18 keV and 100 ps X-ray pulse length with X-ray wavelength 0.689A. The laser configuration was set at 267 nm. We collected measurements with time delays ranging from – 300ns to 1µs. For our measurements we used varying capillary thicknesses (from 100 um to 500 um), and the jet system. To avoid radiation damage, we allowed lateral translation of the capillary. Static references collected: solids as XRD, bulk solution of the hydrogel with WAXS.

Deviation from the Proposal

For the TR-WAXS studies we directly excited tryptophan as chromophore and prepared it in the hydrogel with and without complexing to transition metals. Due to lack of time we weren't able to setup the X-ray

spectrometer and to perform the TR-XES experiments on the transition metal edges. On our last day of the beamtime, the laser performance dropped, therefore we performed static WAXS measurements for references.

Data Analysis

Data analysis is widely progressed. Correlating the changes in intensity with time we observe fast changes at lower q region which is associated with fast rearrangement within the hydrogel network and inter-layer dynamics. This effect is propagated throughout the gel. The full analysis of the TR-WAXS patterns relies on the complete investigation of the WAXS scans and a good modelling of the samples using protein simulation programs. We are currently in the process of generating the simulations of the protein hydrogel chain and comparing it with our TR-WAXS data (Fig 1(b)).

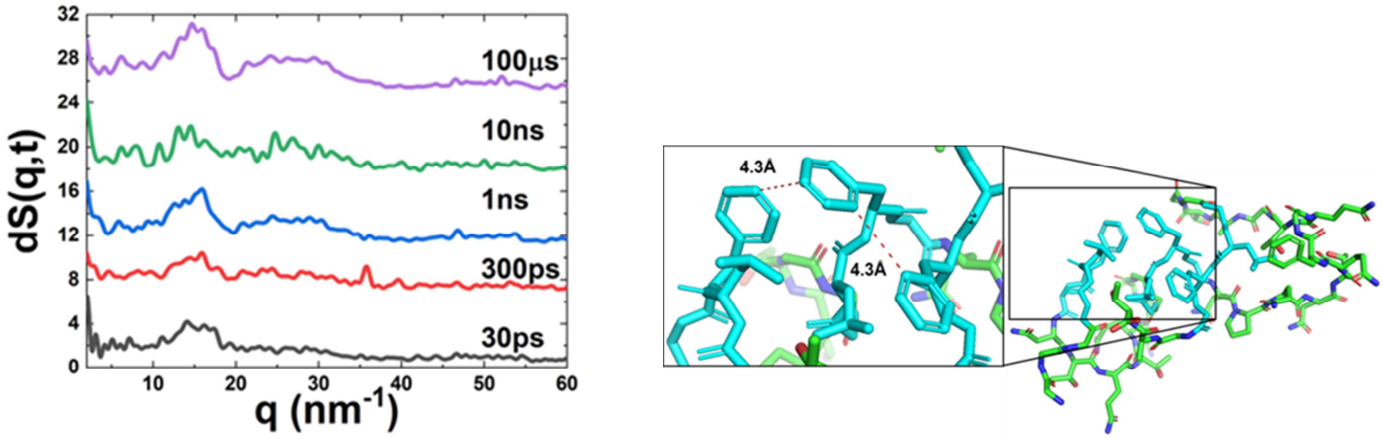

Fig 1:(a) (left side) Difference map of the TR-WAXS curves of protein hydrogel .(b)(right side) Computational simulation of the hydrogel structure demonstrating the inter-layer dynamics.