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# Molecular fluid dynamics description of Rheo-NMR

Abnormal protein aggregation is a hallmark of Alzheimer's disease and numerous other neurodegenerative disorders. Despite tremendous interest in pathogenesis of such diseases, no existing method can capture initial protein aggregate nucleation and subsequent growth at atomic resolution in real time.

To fill this gap, we have recently established high-sensitivity rheological NMR ("Rheo-NMR") spectroscopy that enables us to detect atomic-level structural changes of a protein during amyloid formation in real time (Anal. Chem., 2017, 89). By using the newly developed apparatus, we are able to detect site-specific structural information on amyloidogenic proteins during their amyloid formation in situ, thereby gaining insight into the mechanism underlying amyloid nucleation at atomic resolution.

However, NMR experiments do not provide a truly visual **picture** of protein motion under shear. Nevertheless, we are keen to understand what is actually going on inside the NMR tube during a Rheo-NMR experiment.

Therefore, we are using molecular dynamics simulations to study the motion of protein particles in a simple shearing flow. We are also starting to study the fluid itself numerically by computational fluid mechanics.

Connecting fluid mechanics, biomolecular simulations, and experiments applying shear flow in situ appears to be a promising strategy to understand protein motion, dynamics, and deformation under shear.

References:

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Walinda E. et al., Biochim. Biophys. Acta Gen. Subj., 2019, in press.

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