Formation mechanism of SiO_2-protein composites unravelled by in situ fast SAXS at 20 fps

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A quantitative understanding of aggregation mechanisms leading to the formation of inorganic nanoparticles (NPs) and protein composites in aqueous media is of paramount interest for colloid chemistry, biomineralization or the design of biomedical devices and sensors. In particular, the interactions between silica (SiO_2) NPs and lysozyme (LZM) have attracted attention because silica NPs readily form in natural settings (e.g., biosilification by diatoms, sinter formation in hot springs) and they are key components in numerous technological applications. In turn, LZM is well-known to adsorb strongly to silica NPs, while at the same time preserving its enzymatic activity (e.g., antibacterial properties).

The inherent nature of the aggregation processes leading to NP-LZM composites involves structural changes at length-scales from few to hundreds of nanometers but also time scales << 1 second. To unravel these we used *in situ* synchrotron-based small-angle X-ray scattering (SAXS) and followed the subtle interparticle interactions in solution at a time resolution of 50 ms/frame (20 fps). A complex scattering model was developed, and applied to the SAXS data to unravel mechanistic understanding of LZM induced aggregation of ~5 nm diameter silica NPs. The relative scattering contrast of LZM alone was insufficient to assess its contribution to the scattering pattern, and only the NP component could be followed directly. However, we show that if the size of silica NPs is matched by the dimensions of LZM, the evolving scattering patterns contain a unique structure factor contribution originating from the presence of LZM. The numerical analysis of this structure function allowed us to extract structural information on the deformation of lysozyme molecules during aggregation, as well as to derive the mechanisms of composite formation. The details of the model can be found in [1].

[1] https://github.com/tomaszstawski/SilicaLysozymeSAXS