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Dynamics of Calcium caseinate in H₂O or D₂O studied by Quasi-Elastic Neutron Scattering (QENS)

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Producing meat analogues using calcium caseinate is an intermediate step to reduce carbon emission and improve animal welfare. Depending on the drying methods of the powder, 30% w/w spray-dried calcium caseinate (SCaCas) forms pronounced fibrous structure under shear and heat of 50°C, while roller-dried calcium caseinate (RCaCas) does not¹. Solvent plays a role in the fibrous structure as well. When SCaCas is prepared with D₂O, the formation of fibrous structure is not possible while RCaCas shows anisotropy in the final structure². We hypothesize that drying methods and solvent environments affect the hydration behaviour of the protein powders.

To systematically study the dynamics of calcium caseinate, we performed QENS experiments on both SCaCas hydrated with H₂O (SH) or D₂O (SD) and RCaCas with H₂O (RH) or D₂O (RD). Samples with a hydration level of 0.4g/g dry powder were measured with an energy resolution of ~17.5 μ eV and Q-range of 0.5~1.7 $\text{\AA}^{-1}$.

Mean Square Displacements (MSDs) were extracted by fitting the elastic window scans with Gaussian approximation and is shown in figure 1. The 'dynamical transition' temperature of the SH is the highest (250K), and its slope above 250K the steepest. Results suggest, for RCaCas, the activation energy for protein dynamics is insensitive to solvent. While for SCaCas, the protein dynamics is the same as RD when hydrated with D₂O, but more energy is needed to induce dynamical transition when hydrated with H₂O. Plus, the water dynamics of SH is more active comparing to the rest.

The full energy spectra are fitted with the sum of a Delta function, a Lorentzian function and a linear background. The Full Width Half Maximum (FWHM) of the Lorentzian is fitted with the Singwi-Sjölander model to describe the motions of water molecules. The translational diffusion coefficient (D_t) and residence time (τ_0), plotted in figure 2, were compared between samples at 293K (room temperature) and 320K (50°C). The D_t of both samples increased with increasing temperature, with RH displaying a slightly higher increase (from 0.15 to 0.30 $\text{\AA}^2/\text{ps}$, compared to 0.17 to 0.27 $\text{\AA}^2/\text{ps}$ for SH). As for τ_0 , both samples decreased with increasing temperature. In contrast to bulk water, whose τ_0 is typically 1ps, the water molecules are quite confined to the protein surface, even at elevated temperature. The difference between SH and RH may be attributed to the differences in initial powder morphology and conformational changes in structure at a higher temperature.

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References:

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