Feature-guided SANS analysis to map micellar phase space

Ashley P. Williams [a], E. Wouter Grünewald[a] and Viviane Lutz-bueno[a]

[a]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, Switzerland

ashley.williams@psi.ch

Surfactants self-assemble into a rich variety of micellar structures governed by molecular interactions, solvent conditions and even external stimuli. As a result, identifying micelle structure is still heavily dependent on trial-and-error approaches, with significant cost and risk associated with custom synthesis and formulation. Small-angle neutron scattering provides detailed insight about nanostructure, and with increasing popularity of high-throughput, fluidic approaches to generate large datasets, the bottleneck shifts from measurement to analysis. Within a few hours, hundreds of scattering patterns can be acquired to map micelle structure to surfactant composition and identify synergistic interactions that drive micellar transitions.
In this work we utilise a feature-guided algorithm that exploits changes in low- q gradients, to determine which model parameters should be adjusted. Since micellar transitions are smooth, the initial parameters for one composition is closely related to next, constraining the fitting algorithm and enabling rapid analysis of detailed phase maps. This approach facilitates the generalisation of models and enhances the accessibility and the utility of these information-rich experiments. We exploit this methodology to investigate self-assembly as a result of hydrogen bonding interactions **[1]** .

Keywords:
Small-angle neutron scattering, Self-assembly, Phase mapping, Feature-guided fitting

References:

[1] Viviane Lutz-Bueno, Ashley P. Williams, *Hydrogen bonding exacerbates viscoelasticity of amino acid– and betaine surfactant self-assemblies,* Journal of Colloid and Interface Science **2026** , 704, 1, 139382, https://doi.org/10.1016/j.jcis.2025.139382.