Kinetic Pathways in Self-assembled Soft Matter Systems: applications of synchrotron TR-SAXS

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The kinetic pathways regulating the self-assembly of molecules into well-ordered nanostructures such as micelles, membranes and larger complexes are still not understood. Many processes occur far from thermodynamic equilibrium and occurs on microseconds-milliseconds time scales that until now have been too fast for most experimental techniques. For computer simulations, however, we face the opposite problem; the dynamics of self-assembled systems is generally too slow for studies with accurate molecular precision due to the large number of atoms involved. Time-resolved small-angle X-ray/neutron scattering (TR-SAXS/SANS) is powerful technique[1] that allows kinetics processes such as nucleation processes[2,3] and morphological transitions[4,5,6] to be followed with structural resolution over time scales starting from microseconds -milliseconds. Although the capabilities of the TR-SAXS technique at synchrotrons, such as at ID02 at ESRF, have undergone a dramatic improvement over the last decade or so, studies of self-assembly are often challenging due to difficulties in triggering the process and probing the process short time scales. Often stopped-flow apparatus is used but it is limited to milliseconds kinetics. Alternatively, light[7], in particular lasers, offer a convenient way to study faster processes but is again limited in the variety of suitable systems. Another challenge is the interpretation of scattering data obtained from a kinetic process which often contains highly non-equilibrium structures with a variety of morphologies and large polydispersities, In. this context, computer simulation is very useful but requires suitable methods to be able to quantitatively compare with data obtained from scattering techniques.

In this presentation, we shall show some examples of insight into surfactant assembly and membrane solubilization studies obtained using TR-SAXS and aided by computer simulations. We will discuss triggering methods (stopped-flow and light-induced) and show how combination with computer simulations give insight into mechanism of self-assembly.

References

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