Analysis of Small-angle Scattering Data from Block Copolymer Micelles using Models Based on Monte Carlo Simulations

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Numerous studies of block copolymer micelles formed in selective solvent by scattering methods have been published in the literature. In order to extract information on the structure of the micellar core and corona, modelling is required. Recently, there has been a large progress in the model expressions available for the analysis of such scattering data. The expressions are based on results from Monte Carlo simulations on models with a compact core and a corona of interacting, self-avoiding chains. During the simulations, both scattering form factors and the real-space structure are sampled, so that various semi-empirical expressions can be tested. When established, these expressions can be used in the analysis of experimental scattering data. An overview of the developments is given and the application to micelles of the diblock copolymer Brij700 (C_{18} EO_{100}) in water (D_2O) solution is presented. The micelles consist of a hydrophobic core surrounded by a corona of PEO chains in contact with the solvent. SAXS and SANS experiments are combined to provide complementary information. Both the effect of concentration and temperature are investigated, where the latter parameter induces a change of solvent quality for the PEO chains.

Keywords: small-angle scattering, polymer, theory