DANNALAB

Application note 0004

Structure of SDS micelle

Structure of SDS micelles in aqueous environment

Introduction

Sodium dodecyl sulphate (SDS) is a strong anionic surfactant with formula $NaC_{12}H_{25}SO_4$. The surfactant properties of SDS are derived from its ability to form globular core-shell micelles in an aqueous solution above the critical concentration level (CMC).

One of the important applications of SDS in structural biology is the use of the micelle surface to mimic the native lipid bi-layer environment.

In particular, DANNALAB conducts experiments to simulate the binding and aggregation of naturally unfolded proteins using SDS micelles as a model structure.[1]

Reliable methods of micelle structure reconstruction are therefore necessary to investigate the details of protein binding to SDS.

This application note describes the part of the study aiming to reconstruct the structure of SDS micelles in aqueous solution at different pH levels.

Experiment

Samples of SDS dispersion were prepared from pharmaceutical grade SDS powder (mfg Sigma) by mixing with a stirrer for 24 hours at 40°C and filtration. SAXS data were collected from a 1% wt aqueous dispersion of SDS (Figure 1).

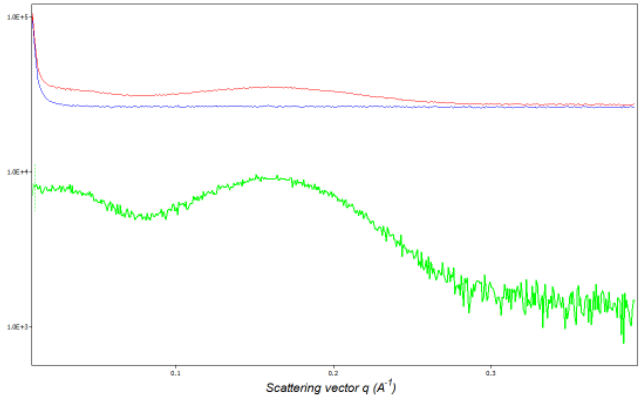

Figure 1. SAXS pattern of SDS dispersion is shown in red, pattern of water is shown in blue and their differential is shown in green.

Results

First, the data were analysed by reconstructing the PDDF distance-distribution function*.

Figure 2 shows the reconstructed function.

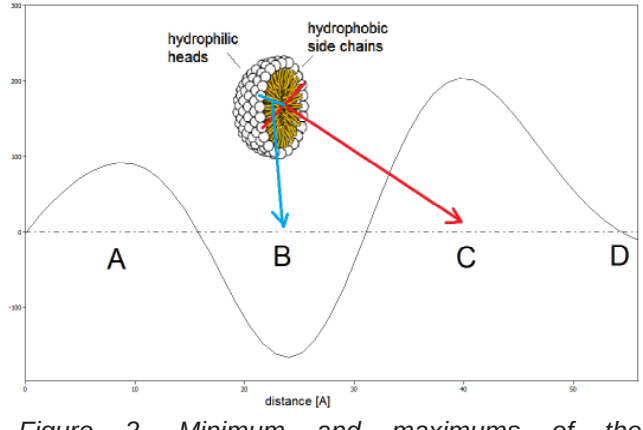

Figure 2. Minimum and maximums of the reconstructed PDDF function indicate the characteristic distances within the particle.

Point C on Figure 2, at ~41 (A), may serve as an estimate of the average distance between the opposite hydrophilic groups in the micelle. Point D, at ~55 (A), indicates the maximum distance within the particle. Point B is the length of the average of all vectors inside the micelle connecting parts with positive (hydrophilic) and negative (hydrophobic) relative scattering densities.

The second analysis method applied to the same experimental data used the fitting of the experimental differential curve by model based on the double core-shell structure. The two- shells model was introduced to more accurately mimic the outer part formed by hydrophilic heads. In this case, parameters of core and shells – size, scattering contrast and polydispersity – were refined to obtain the best fit with the differential pattern (Figure 3).

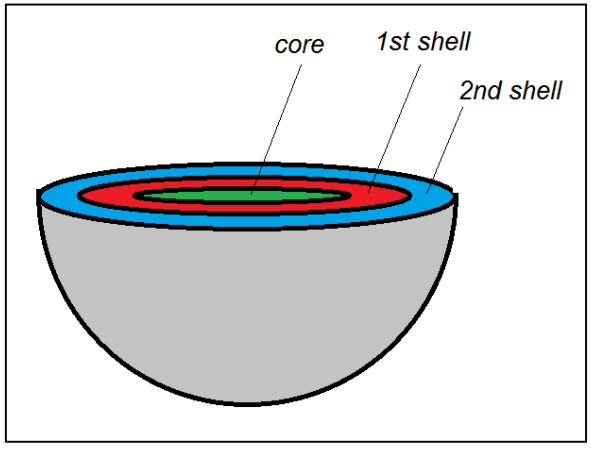

Figure 3. Model of micelle with a core-shell structure.

Refinement of core-shell model returned the following parameters:

Core: radius = 15.5[A], σ=13%, ρ=-3.8
1st shell: thickness = 3.8[A], σ=9%, ρ=2.8
2nd shell: thickness = 1.9[A], σ=22%, ρ=5.9

The values above refer to σ as polydispersity and ρ as relative (to water) scattering contrast.

The resulting distribution of scattering contrast in micelle associated with relative (to water) electron density is also depicted in Figure 4.

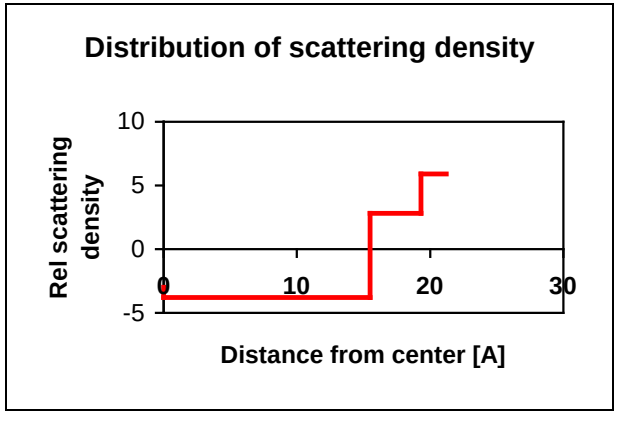

Figure 4. Distribution of scattering density as a function of distance from the particle centre.

The average distance between the centres of opposite hydrophilic groups calculated from the centre of the second shell is equal to ~40.5 [A].

Therefore, both methods result in comparable values for particle size.

The advantage of the first method is flexibility and independence from the model. The second method demands the introduction of a realistic model, but fitting by model brings actual numerical values to the refined parameters.

Reference

[1] Application note DANNALAB 0002

** PDDF is a self-correlation function of relative scattering density within the particle. Maximums of PDDF function show the most populated vectors inside the particles connecting the areas with the largest scattering density.*