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SANS Model

SANS is a well-established technique for determining the structures of self-assembled amphiphilic molecules. It essentially provides differential scattering cross-section per unit volume as a function of wave vector transfer (Q), which for monodispersed particles can be expressed as[1,2]:

$$\frac{d\Sigma}{d\Omega}(Q) = nP(Q)S(Q) + B \quad (1)$$

Where n is the number density of the scatterers. $P(Q)$ is intra-particle structure factor, which is basically the orientational average of the square of the form factor$F(Q)$. The shape information of the particles is reflected in the intermediate Q-range, where for standard shapes such as cylindrical it has $1/Q$ dependence, $1/Q^2$ for vesicles and $1/Q^4$ for multi-lamellar vesicles. $S(Q)$ is the Fourier transform of the radial distribution function $g(r)$ for the mass centers of the particles and is known as inter-particle structure factor. $P(Q)$ is decided by the shape and size (structural parameters) of the scatterers while $S(Q)$ provides information about interaction among them. For a dilute system, where the interparticle distance between the scatterers is large enough, $S(Q)$ may be considered as unity. Finally B represents a constant term corresponding to the incoherent background originating mostly from the hydrogen present in the system.

For vesicles following equation for core-shell model having inner radius R and thickness dR can be used[3]

$$F(Q) = \frac{16\pi^2}{9}(\rho_p - \rho_s)^2[(R+dR)^3 \frac{sinQ(R+dR) - Q(R+dR)cosQ(R+dR)}{Q^3(R+dR)^3} - R^3 \frac{sinQR - QRcosQR}{Q^3R^3}]^2 \quad (2)$$

Where ρ_p and ρ_s are the scattering length densities of particle and solvent, respectively.

For prolate ellipsoidal particles, P(Q) can be expressed as

$$P(Q) = \frac{16\pi^2}{9}\left(\rho_p - \rho_s\right)^2 \left(ab^2\right)^2 \int_0^1 \left[F(Q,\mu)\right]^2 d\mu \tag{3}$$

where the functions are given by

$$F(Q,\mu) = \frac{3(\sin x - x\cos x)}{x^3} \tag{4}$$

and $x = Q[a^2\mu^2 + b^2(1-\mu^2)]^{1/2}$, where a and b=c are, respectively semi-major and semi-minor axes of prolate ellipsoid (a>b=c). The variable μ is the cosine of the angle between the directions of a and Q.

For charged micellar system, S(Q) is usually calculated by using the Hayter and Penfold analysis under rescaled mean spherical approximation (RMSA), which assumes screened Coulomb interaction between the charged particles.[4] For the two populations (micelles and vesicles) present in the system, total scattering intensity is calculated by summing up the scattering contributions from two scatterer entities. The % volume fraction of the micelles is then calculated from the pre-factor of the scattering term corresponding to the micelles.

The aggregation numbers of the monomers in the mixed micelles having prolate ellipsoidal shape were calculated using following eqn[5]:

$$N = \frac{4\pi ab^2}{3\overline{V_m}} \tag{5}$$

Here, V_m can be calculated from their respective average surfactant monomer volumes, V_{mSDS} and V_{mL121}

$$\overline{V}_m = (V_{mSDS} \times X_{SDS}) + (V_{mL121} \times X_{L121}) \quad (6)$$

Where X_{SDS} and X_{L121} are the mole fractions of SDS and L121, respectively. $V_{mSDS} = 350.2$ Å^3; $V_{mL121} = 7100$ Å^3.

References

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