Structure of bicelle formed by mixed surfactants

Kenji Kubota*[1], Kousirou Taya[1], Rio Kita[2], Kenji Ochiai[1] and Kaori Wakamatsu[1]
[1]Faculty of Engineering, Gunma Unive., Kiryu, Gunma 376-8515, Japan
[2] Supramolecular Science Laboratory, RIKEN (The Institute of Physical and Chemical Research), Wako, Saitama 351-0198, Japan

Introduction

Bilayered mixed micelle, known as bicelle, is a molecular assembly in which the long-chain phospholipid-rich disc-shaped bilayered structure is stabilized by the regular alignments of surfactant (short chain phospholipid or detergent) on the periphery of the disc. Therefore, bicelle is a suitable model membrane system and is useful for the physicochemical and biochemical studies of membrane proteins. CHAPSO is a twitterionic detergent having the steroid group similar to bile salts, and its solubility is fairly high with CMC being ca.8mM. Though it has generally been expected that the mixture of DMPC and CHAPSO forms bicelles, the structure of phospholipid-CHAPSO mixture has not been studied in detail. The detailed structure of bicelles containing CHAPSO was determined by SAXS measurements combined with model calculations of scattering functions taking into account the spatial variation of electron densities.

Experimental

L-α-Dimyristoylphosphatidylcholine (DMPC) used for the preparation of the mixed micellar solutions were purchased from Avanti Polar Lipids Inc. (Alabaster, AL) and was used without further purifications. Detergent, (cholamidopropyl) dimethylammonio-2-hydroxy-1-propanesulfonate (CHAPSO) was obtained from DOJINDO (Kumamoto, Japan), and was of 96 % purity. The respectively dispersed solutions of DMPC and CHAPSO were mixed to make the final solutions for the measurements by employing ultrasonication. Dynamic light scattering measurements were also carried out using a homemade spectrometer and an ALV-5000 multiple-tau digital correlator to obtain the correlation functions of scattered light $g^{(2)}(t)$. Vertically polarized Ar ion laser operated at the wavelength of 488.0 nm was used as the incident beam. Hydrodynamic radius was calculated by using the Einstein-Stokes equation. Small angle X-ray scattering measurements were performed by BL-10C station of KEK-PF (λ_0 = 0.149 nm). All the measurements were carried out at 30°C [1].

Results and Discussion

Typical result of the scattering function (q = 1.0, 50 mM, and at 30°C) is shown in Fig. 1. Here, the solid curve is calculated for a model structure of DMPC/CHAPSO bicelle by introducing the spatial variation of electron densities (details are described below). By the method of Guinier plot, radius of gyration R_g was determined at the small scattering vector region. The obtained R_g was 3.39 nm for Fig. 1. In the present case, it was necessary to simulate the scattering function based on the model structure of the assemblies to determine the

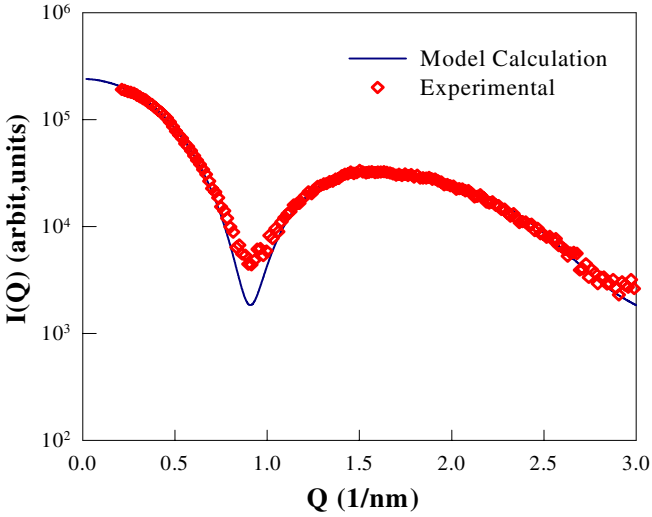

Fig. 1 Scattering profile (q = 1.0, 50 mM at 30°C).

detailed three-dimensional structure. Scattering functions were calculated for several model structures, such as a bicelle (bilayered disc) with three or five layers of electron density variation along the disc normal and periphery (rim), rotational ellipsoid, sphere (micelle or vesicle), rod (or cylinder), and so on. The solid curve in Fig. 1 is obtained for the model of the bicelle structure with five layers of electron densities. The fitting is quite good with this model, and calculations with other model failed to give such an agreeable result. The resultant thickness of the bicelle composed of DMPC and CHAPSO is ca. 4.4 nm in good agreement with the reported values for the lamellar thickness. Such a spatial profile suggests that the bilayered assembly of DMPC is edge-stabilized by two CHAPSO molecules aligned in the direction of the disc normal, and that CHAPSO molecules are located also in the bilayered surfaces with the sterol pseudoplane oriented parallel to the surface. The three OH groups of sterol ring which are located on one face of the pseudoplane are considered to direct toward the outside of the bicelle with the other (hydrophobic) face oriented toward the hydrophobic interior. That is, the mixture of DMPC and CHAPSO forms the commonly expected bicelle structure at q = 1.0. This model picture is similar to that of phospholipid/bile salt mixture, although the packing state of CHAPSO molecules in the present bicelles differs from those proposed so far.

References

[1] K.Taya, K. Kubota, K. Ochiai and K. Wakamatsu, Trans. M. R. S. Japan, in press (2002).

* kkubota@bce.gunma-u.ac.jp