Bilayer perforations and self-assembly of spatial networks in solutions of ionic surfactants

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For many ionic surfactants and phospholipid systems, experiment and computer simulation show transitions from nonperforated flat bilayers and vesicles to the perforated structures and to the spatial networks of wormlike aggregates [1-4]. Substantial change in the system's behaviour caused by such transitions proves important in many fields ranging from production of oil to bioengineering and design of 'smart' materials.

A suitable model of a perforation in a bilayer is a hole with a toroidal rim, Fig. 1A. When three such holes come close, they form structural element that models a junction between three cylindrical aggregates, Fig. 1B: a piece cut from the planar bilayer by a curvilinear triangle framed by three identical pieces of toroidal rims.

In this work we apply the molecular thermodynamics model of the aggregation free energy [5] to study relative stability of the aggregates of different shapes. For toroidal geometry, an accurate analytical approximation gives the electrostatic contribution to the free energy. We illustrate the stabilization of perforations in bilayers and describe the sequence of shape transitions induced by adding salt, including formation of bicontinuous structures and branched or nonbranched wormlike micelles for ionic surfactants.

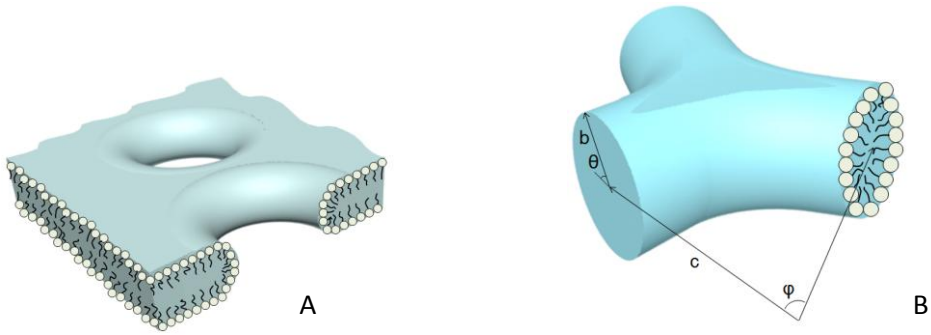

Figure 1 A piece of perforated bilayer (A) and Y-shaped junction between three cylindrical micelles (B). *c* and *b* are the major and minor radii, respectively, of the toroidal element of the junction.

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