Vesicles for encapsulation: a coarse-grained mean-field theory study

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Abstract

Polymer vesicles show great potential as vehicles for the encapsulation and delivery of active chemicals due to their durability and low permeability. We focus here on two problems of current experimental interest: fixing the size of vesicles through the use of novel multiblock polymers, and encapsulating chemicals inside the vesicle wall rather than in its aqueous centre. These systems are appropriate for the capture of hydrophilic and hydrophobic compounds respectively.

First, we demonstrate in a coarse-grained mean-field model (self-consistent field theory) that copolymers with four sections (tetrablocks)[1,2] can, in contrast to simple diblocks, form vesicles with a preferred radius. We then investigate how the polymer properties must be varied in order for this target structure to form (see Figure 1).

Second, we use a similar approach to study the properties of oil droplets encapsulated in amphiphile bilayers, and investigate how changing the nature and size of the oil molecules can control the properties of the droplet. Our numerical results are compared with a simpler model based on the tension of the membrane.

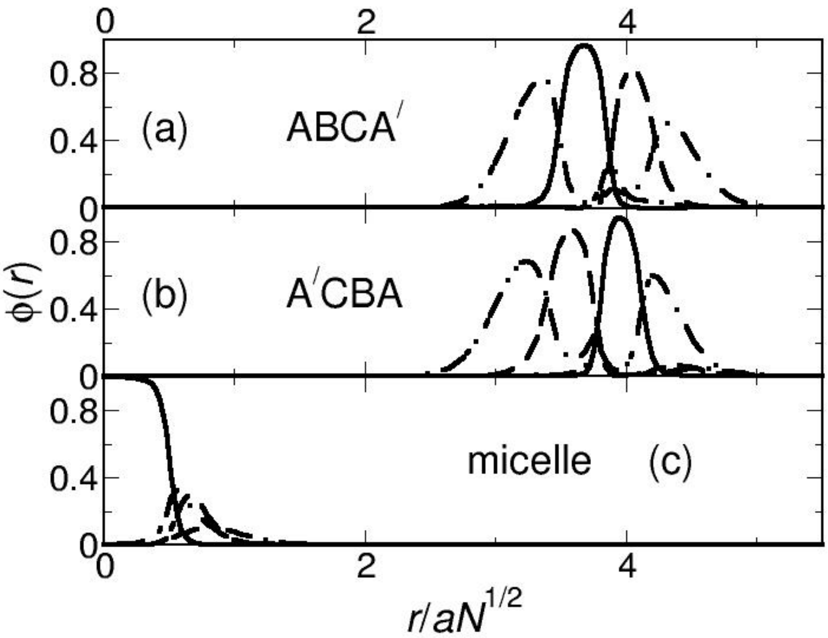

Figure 1: Cuts through the density profile of ABCA tetrablock aggregates: (a) vesicle (b) inverted vesicle and (c) micelle. Hydrophobic blocks are shown with full or dashed lines, hydrophilic blocks with dot-dashed lines. Polymer parameters are varied to form structure (a), which has a preferred curvature.

[1] E. D. Gomez, T. J. Rappl, V. Agarwal, A. Bose, M. Schmutz, C. M. Marques and N. P. Balsara, *Macromolecules.* **38**, 3567 (2005).
[2] A. K. Brannan and F. S. Bates, *Macromolecules.* **37**, 8816 (2004).