

Typical abstract:

Topic 3: Advancements in materials testing and characterization

## A Brownian Dynamics Study of the Effect of Interfacial Curvature on the Adsorption of Copolymer Stabilized Nanoparticles at Liquid-Liquid Interfaces

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Block copolymer-stabilized nanoparticles placed in the presence of a curved oil-water interface are described using Brownian Dynamics simulations. The contact angle, the order parameter and polymer density across the interface are used to assess the effect of a given block copolymer composition on the adsorption at the liquid-liquid interface. We study the contact angle of block copolymer stabilized nanoparticles at different block copolymer compositions (see Figure 1). We find that the contact angle for a block-copolymer stabilized nanoparticle is affected by the curvature of the oil-water interface. This is a departure from earlier results of Komura et al. [1], where the contact angle of a solid particle at a curved interface obeys the Young's formula for contact angle, in which case it is independent of the interfacial curvature. A part of the change of contact angle results from the increase of the radius of gyration of the nanoparticle due to the presence of the block copolymer. Furthermore, an investigation of the structure of the block copolymer and its distribution across the interface (see Figure 2) reveals changes as the curvature of the interface is changed, and those changes are reflected in different contact angle values.

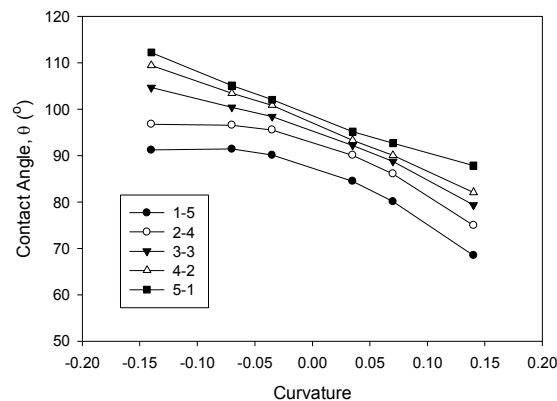


Fig. 1: Contact angle versus curvature for five different block copolymer compositions attached to the nanoparticle.

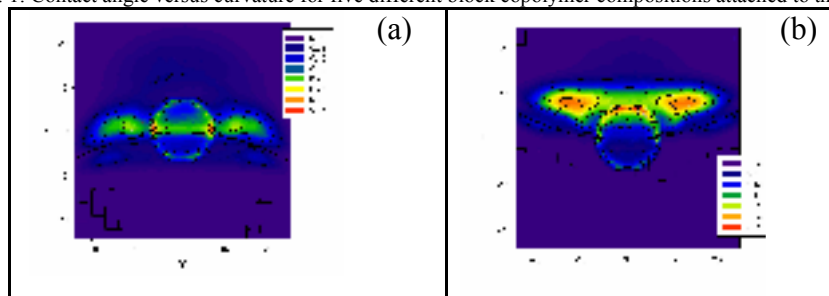


Fig. 2: Contour plots of a block copolymer stabilized nanoparticle at two extreme curvature values (a) and (b) for the same block copolymer composition.