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Monte Carlo simulation of a mixture of carbon nanotubes and surfactants in aqueous solution

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Abstract – In this work, a Monte Carlo simulation of carbon nanotubes and surfactants in aqueous solution has been performed. By using a simple bi-dimensional model, many features of real systems are described. The analysis of equilibrium configuration has been done by means of the structure function. In low concentrations the surfactants strain around the nanotubes, as forming circular micelles. For higher concentrations, they form aggregates like deformed lamellas and vesicles. This suggest that the nanotubes deform the aggregates when penetrate them. The dissociation of carbon nanotubes clusters occurs for surfactant concentration above CMC.

Carbon nanotubes (CNT) exhibit properties that are of huge interest in industry and most different scientific areas [1]. Indeed, the countless theoretical possibilities of this material make it a subject of intense scientific research [2]. A major hindrance to meet this goal is the aggregation of nanotubes in bundles due to strong van der Waals forces [3]. A possible way to dissolve these bundles is the use of surfactant molecules adsorbed on nanotubes surface [4,5]. In the present work, by using Monte Carlo simulations, we have found the equilibrium structures of nanotubes and surfactant molecules in aqueous solution. Our model is simulated in a continuous 2-dimensional space. We have performed simulations for several temperatures and surfactant concentrations. The equilibrium structures were analyzed by means of the radial distribution function. At low concentrations, strained surfactants aggregate on the nanotube surface. At medium concentrations, surfactants aggregate in lamellas and at higher concentrations they tend to form vesicles. Our results suggest that nanotubes deform the surfactants aggregate when penetrate them. This occurs due to the fact that the nanotubes are as big as surfactants aggregates. Dissociation of CNT clusters occurs above critical micellar concentration. This suggests that the determinant factor for this dissociation is the capacity of the amphiphiles to form big aggregates.

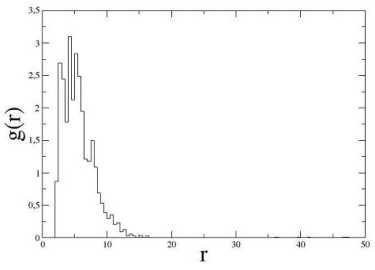

Figure 1: Radial distribution function of 20 amphiphiles and 1 carbon nanotube at reduced temperature T=3. Amphiphiles aggregate around the nanotube surface, like a circular micelle.

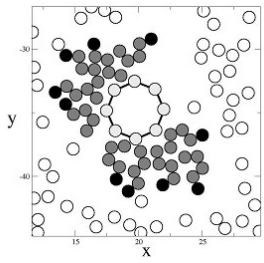

Figure 2: A picture of the circular micelle corresponding to the **figure 1**.

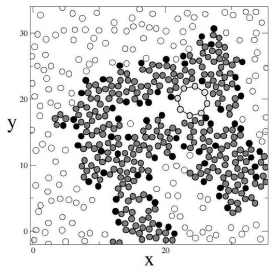

Figure 3: A vesicle-like cluster. This picture corresponds to the simulation of 1 nanotube in aqueous solution and much higher amphiphilic concentration.

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