MC SIMULATION OF WATER MENISCUS IN NANOCAVITIES

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The study of properties of water confined in complex systems with nanometric dimension is relevant to many important processes ranging from industrial applications (water membranes, filtering, etc) to biological processes (protein folding, ionic transport through membranes,...) [1]. In these systems, the water behavior is determined by the large surface/volume ratio as well as the non negligible interaction between water and container. Changes in thermodynamics, phase behavior and molecular mobility of water have been observed upon confinement [2].

In particular, we are interested in the behavior of the water menisci formed in different nanometric cavities. For example, in closed geometries, we have studied the structural effects of the capillary forces on viruses collapse during the final stage of desiccation see Figure 1. [3, 4]. Another interesting problem, with technological relevance, is how the formation of a nanometric water menisci may modify the light propagation in photonic waveguides formed by void structures (as inverse opals) and may change properties like the refraction index. These changes open a way for the design of photonic materials with controllable properties (for instance, under control of relative humidity).

In this paper we will show how lattice gas models used to mimic water behavior and solved by Monte Carlo calculations Figure 2[5] together with electromagnetic and finite element structural force calculations may be used to tackle a large variety of these interesting problems, as those mentioned above.

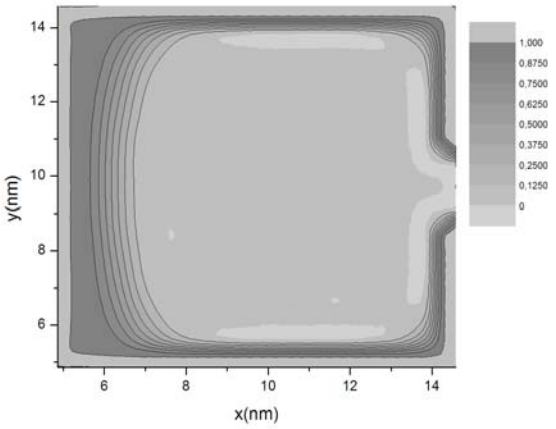

Figure1. Last stage of the desiccation process for a simulated model virial capsid, over an average of 1000 viruses

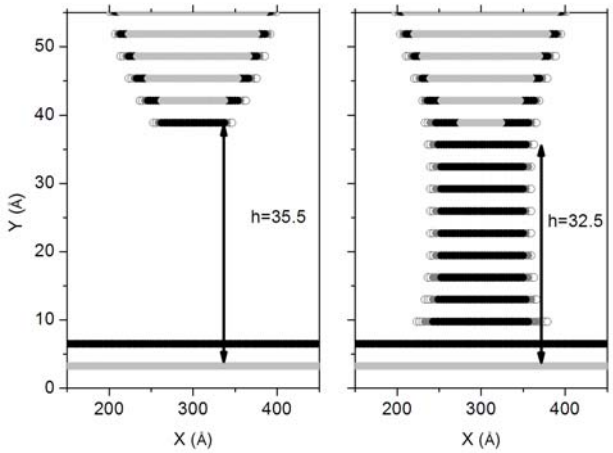

Figure2. MC simulation of a water bridge formation between an AFM tip and a flat surface, both hydrophilic. Formation of the water nano-neck takes place at a distance of 33A° for the set of parameters considered (T=294.62K, RH=70%).

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