Poster

MC SIMULATION OF WATER MENISCUS IN NANOCONTAINERS: EXPLAINING THE COLLAPSE OF VIRAL PARTICLES DUE TO CAPILLAR FORCES.

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The study of properties of water confined in complex systems is relevant to many important processes ranging from industrial applications (water membranes, filtering, etc) to biological processes (protein folding, ionic transport through membranes,...) [1]. Changes in thermodynamics, phase behavior and the molecular mobility of water have been observed upon confinement [2]. These changes are strongly dependent on the nano-container properties. In particular, very recently [3-4] we have reported, using atomic force microscopy (AFM), that remarkable structural modification takes place during the desiccation processes on individual particles of the bacteriophage ϕ29 and the minute virus of mice (MVM). In both cases the genomic DNA was ejected from the viral capsid (see Figure 1). However, while the structural integrity of the minute virus of mice was essentially preserved, the ϕ29 capsid underwent a wall-to-wall collapse. These results points towards the important role played by the capillary forces of water confined inside the viruses. In fact, the desiccation process of an empty viral particle (nano-container) is associated to the formation of internal water menisci with shape (exposed area and curvature) determined by the capsid geometry.

In order to study the way in which the water menisci evolves during the desiccation process of viral particles we have simulated the water+capsid system using a lattice gas model that mimics the gas-liquid phase transition in water. This model has been previously used to study the geometry of the water meniscus formed between an atomic force microscope tip and a substrate [5]. Averaged Monte Carlo (MC) simulations of the water meniscus evolution have been carried out for two types of viruses' cavities: an asymmetric one with a single channel and a symmetric one with pores at every fourfold symmetry axis. The MC simulations describe the formation of an asymmetric water meniscus for the virus with a single hole (ϕ29) whereas, for the virus with a symmetric location of the pores (MVM), the water bridge formed is symmetric and capillary forces could cancel one another (see Figure 2). These differences could explain the wall-to-wall collapse noticed for ϕ29 viral capsids. In order to determine these forms, the future work is based on a accurate determination of the water meniscus profile for each step of the desiccation process. Characterization of the profile will be performed by fitting to geometric parameters like Kelvin´s radius [6].

References:

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Figure 1. MVM (Left) and φ29 (Right) viral particles after de-wetting processes with their respective DNA ejected from the capsids.

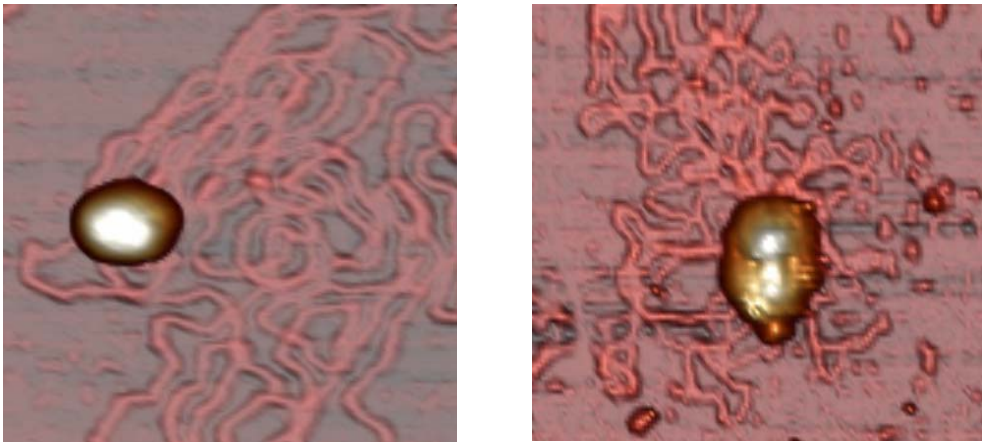

Figure 2. Numerical simulation of a desiccation process for asymmetric (upper panel) and symmetric (lower panel) virus cavities. Monte Carlo steps considered are 200, 600, 800, 1100 (upper panel from left to right) and 200, 400, 500, 700 (lower panel from left to right). Every lattice site with averaged water occupation probability n(i,j)>0.5 is represented with a blue point. Points belonging to the virus cavity are represented with a black line.