MOLECULAR DYNAMICS OF CARBON NANOTUBE-POLYPEPTIDE COMPLEXES AT THE BIOMEMBRANE-WATER INTERFACE

KONSTANTIN V. SHAITAN,* YEGOR V. TOURLEIGH, DMITRIY N. GOLIK
Lomonosov Moscow State University, Dept. of Bioengineering

Abstract. Molecular dynamics simulation of a system consisting of a hydrated lipid bilayer, a nanotube with a cap at one end, and a polypeptide to be pushed through the membrane is reported. This construction is considered to be a delivery vehicle (nanosyringe) which drives the peptide to the membrane surface. Tuning the nanotube (by adding functional groups) one may achieve the selectivity of the nanotube landing area on the cellular membrane. The pressure expulsing the peptide could arise as a result of a chemical reaction that makes the reaction mixture volume increase in the nanotube. As an analogue of the explosive component, blowing Van der Waals spheres are proposed. Different regimes of the penetration are simulated.

Keywords: molecular dynamics; nanotubes; biomembranes; peptides; drug delivery

Methods of molecular dynamics currently are widely applied in the study of the most fundamental topics of natural sciences as well as in nanotechnology research. A molecular device able to selectively inject molecules through the cell membrane is described. This nanosyringe is a nanovehicle, which carries not too big molecules to the membrane (Fig. 1). The molecules are protected by the wall of a carbon nanotube. In the next step, the nanotube interacts with a receptor site on the membrane in accordance with the molecular tuning of the free end of the nanosyringe. Then, the active agent can be shot from the nanosyringe through the membrane structure. The nanosyringe is filled with an olygopeptide and a working medium, which is represented by an active compound increasing its volume due to a chemical reaction. As a model of the microexplosive agent, a set of Van der Waals spheres was taken. The spheres

*To whom correspondence should be addressed. Konstantin V. Shaitan, Bioengineering Department, Moscow State University, Leninskie Gory, 1/12, 119992, Moscow, Russia; e-mail: shaitan@moldyn.org

V.N. Popov and P. Lambin (eds.), Carbon Nanotubes, 233–234.

were enlarging their volumes at a certain rate. Some dynamical aspects of these processes are reported below.

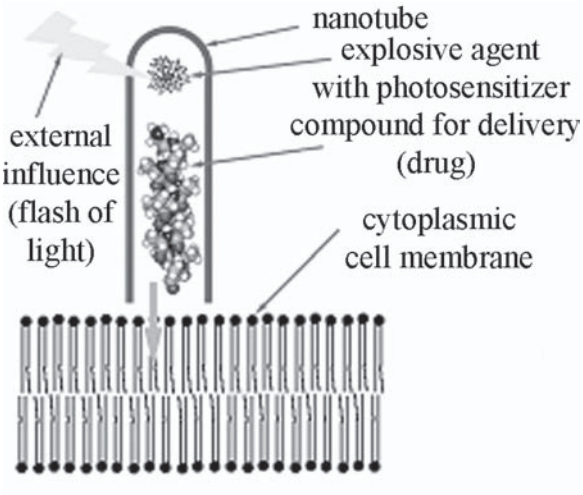

Figure 1. Scheme of the nanosyringe in action.

The uptake of the peptide to the nanotube is energetically favorable and can take place spontaneously. The time of self-assembly at 300 K was estimated as 40 microseconds. Under the shock action, the polyalanine alpha helix greatly changed the conformation (Fig. 2) and partially denaturated. In the model system, the delivery of a compound to the membrane under the action of a nanoexplosion turned out to be possible.

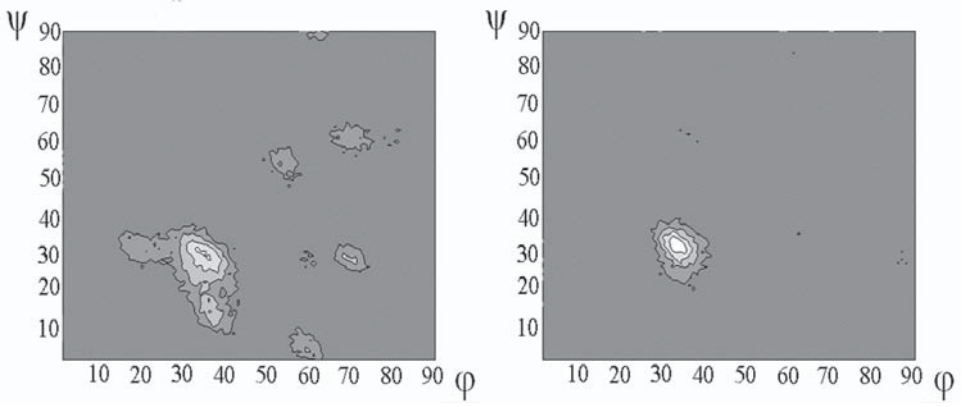

Figure 2. Poincare sections for the φ and ψ angles averaged over all polyalanine residues under the extrusion to the membrane at 13 ps (left) and 26 ps (right) from the beginning of the spheres enlargement.