Nanocomposites and nanomaterials

Interactions between carbon-based nanostructures and biomembranes – computer simulations study

P. Raczynski[1,2], K. Gorny[1,2], Z. Gburski[1]

[1] *Institute of Physics, University of Silesia. Uniwersytecka, 4, Katowice 40-007, Poland.*
E-mail: przemyslaw.raczynski@us.edu.pl

[2] *Silesian Ctr Educ & Interdisciplinary Res, University of Silesia. Chorzow 41-500, Poland.*

Cell membrane is an efficient barrier created by nature to protect the interior of the cell from the outside environment. A significant part of the cell membrane is phospholipid bilayer, the structure consisted of phospholipid and cholesterol molecules. We prepared a model of phospholipid bilayer and indented it using single-walled carbon nanotubes and graphene sheets. Two different CNTs (10, 10) and (12, 12) were taken into account as well as two graphene sheets of different size (9 x 3 nm and 1.5 x 3 nm). The phospholipid bilayer was indented with two speeds: 1 m/s and 2 m/s. All full-atomistic SMD simulations were performed at the physiological temperature. The average force acting on nanotube during membrane penetration versus indentation depth and required work have been calculated.

The damage of the phospholipid bilayer means cell death. Motivated by this we have performed a series of simulations with pulling the nanostructures out of the membrane. In this way we assess the self-sealing ability of the membrane after the extraction process. The relatively small pulling velocities should minimize the impact of the foreign body on the phospholipid bilayer.

Nowadays medicine needs nanoobjects, that can penetrate through the phospholipid bilayer, despite the low permeability of and without damage to its structure. Taking into account the unique properties of carbon-based nanostructures, they seem to be a good candidates.

Figure shows a set of snapshots of the nanoindentation process of the bilayer by (12, 12) nanotube: a) initial configuration, b) CNT reaches polar heads, c) CNT reaches the glycerol backbone, d) CNT reaches the second layer of membrane, e) final configuration.