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ANALIZA EFEKTU ŚCIANKI NA PROCES DYFUZJI NANOCZĄSTEK W MIKROKANALE.

ANALYSIS OF WALL EFFECT ON THE PROCESS OF DIFFUSION OF NANOPARTICES IN A MICROCHANNEL

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Recently, the classical nonslip hypothesis for the tangential velocity of liquid adjacent to the solid surface became questioned for the flow in micro- and nanofluidic devices. The topic is of fundamental interest and has potential practical consequences in many areas of applied sciences. Hence, several experimental and numerical studies were performed to elucidate presence of the molecular-scale slip for the flow of Newtonian liquids in microchannels. It came out that in the most investigated configurations the slip velocity (or so called *slip length*) exists and can be measured.

However, values obtained for the slip length strongly vary from the experiment to experiment,

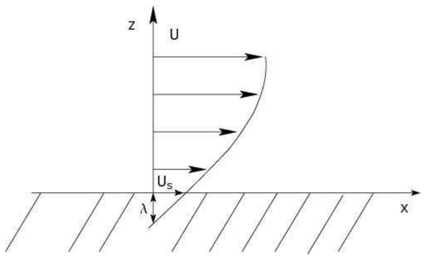

Fig. 1: Navier slip law.

$$\vec{U}_s = \lambda \dot{\gamma},$$
$$\dot{\gamma} = \frac{dU(z)}{dz},$$

$\vec{U}$ − *fluid velocity*,
$\vec{U}_s$ − *fluid velocity at the wall*,
$\dot{\gamma}$ − *shear rate*,
λ − *slip length.*

covering range of several nanometers to several microns [1, 2, 3, 4, 5]. It is partly due to the experimental difficulties in performing accurate velocity measurements of flow at molecular distances from the wall. To avoid problems appearing in reconstructing flow velocity profile in nanometric layers, we propose to evaluate how the slip/non-slip boundary conditions affect behaviour of a Brownian particle performing its chaotic motion close to the wall. According to the theoretical model by E. Lauga and T. Squires [6] the diffusion coefficient of a single colloidal nanoparticle is directly related to the distance from the wall, and the slip velocity. In this work we apply this outcome to determine the slip length from measured and calculated variations of the diffusion coefficient of particles as a function of distance from the wall. For this purpose the effect of the wall on the Brownian motion of nanoparticles suspended in water is examined both in the numerical simulations using molecular dynamics and in the experimental study.

The Brownian diffusion of *24 nm* nanoparticle suspended in water in an infinite channel formed between two quartz walls is simulated by the molecular dynamics code LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). The computations were performed for the square domain of 310.5 nm size and periodic boundary conditions for the two side walls. All interactions between particles were described by the granular potential, which is a modification of the Lennard-Jones potential. Several simulations were performed to evaluate Brownian motion of colloidal particles placed at different distances from the wall. The outcome of the numerical analysis is still not quite clear, our preliminary results suggest absence of the slip velocity. However, due to the well known constrains of the numerical model (short physical simulation time, two-dimensional domain) it may be an artefact. The work is still in progress.

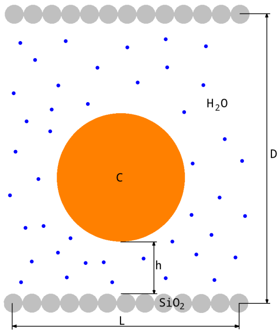

Fig. 2: MD simulation domain (not to scale) with one 24nm colloidal carbon particle suspended in water between to quartz walls. L=D=310.5nm.

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